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GRUCON Code Package Capacities in Creating of ACE Data Files for Monte Carlo Transport Calculations

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Plan of Inter-Comparison Exercise

1. Prepare working ENDF and ACE working libraries from 235U, 238U, 239Pu files, loaded from IAEA-CIELO Web page and processed by PREPRO-2015, NJOY-2016 and GRUCON codes;
2. Compare reconstructed from resonance parameters and Doppler broadened cross sections
3. Compare the effective cross sections derived from the Probability Tables (PT) and Subgroup Parameters (SP), at infinite and 1 barn dilutions, using ACE_UNPACK, ACE_PLOT /V.Sinitsa/, PLOTTAB, PLOTSAVE /D.Cullen/;
4. Run MCNP code for benchmarks, sensitive to shielding in the URR, using identical inputs data but different ACE files for the 235U, 238U, 239Pu nuclides, taking the rest from the ENDF/B-VII.1;
5. Inter-compare Monte Carlo simulation responses for the cases with/without self-shielding;
6. Compare calculated and experimental values.

1. Working Data Libraries

Data libraries, involved in inter-comparison procedure, contain:

ACE-1 library, with

- **U-235** and **U-238** (26Sep2017) **CIELO/ACE** files downloaded from the Web page https://www-nds.iaea.org/CIELO/
- **Pu-239 ACE** file prepared from **Pu-239 CIELO/ENDF** file (original name is Pu239e80b4_5_corDN, as submitted by D. Neudecker on 22 February) through **NJOY-2016** (date of installation 20Sep2017)
- **ACE** files for **56** materials, involved in benchmarks calculations (including thermal polyethylene H(CH2)); they were obtained from the **ENDF/B-VII.1** data by **NJOY-2016** processing code

ACE-2 library, with

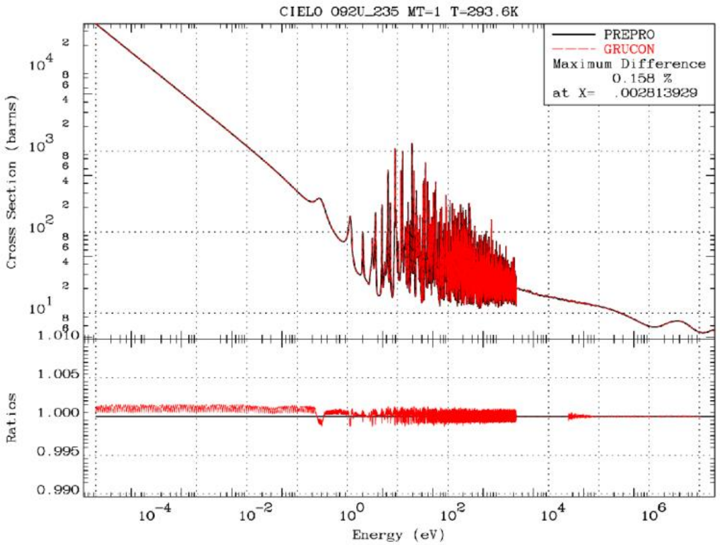
- **56 ACE** files, prepared from the **ENDF/B-VII.1** data by **NJOY-2016** processing code system
- **ACE** files for **U-235**,**U-238** and **Pu-239** prepared from **CIELO/ENDF** files by **GRUCON** code package

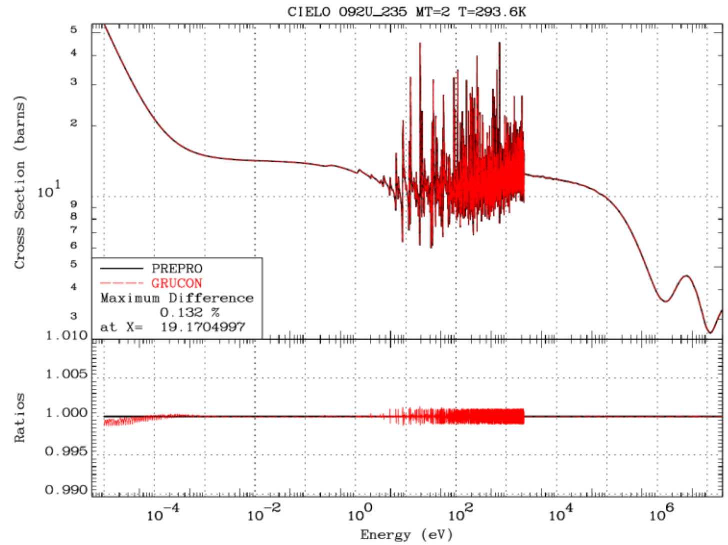
ENDF-PREPRO and **ENDF-GRUCON** auxiliary libraries with point-wise cross sections, reconstruction from resonance parameters and Doppler broadened by **PREPRO-2015** and **GRUCON** processing codes, for **U-235**,**U-238** and **Pu-239 CIELO/ENDF** Files.

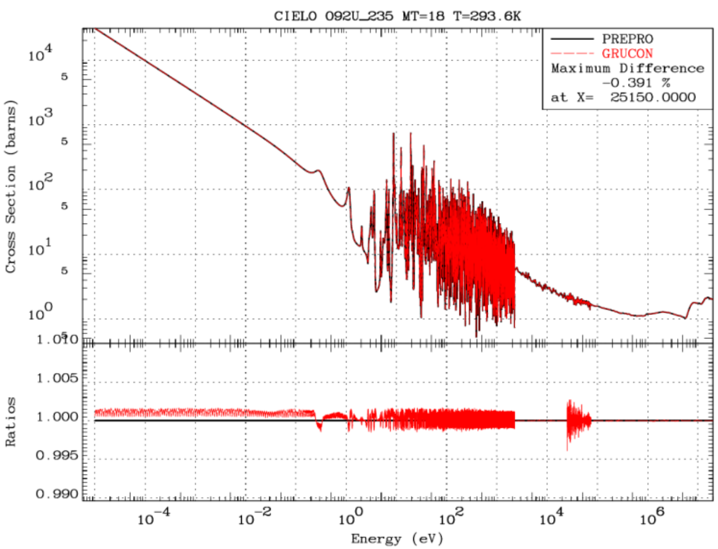
Tolerance parameter: **EPS=0.001**

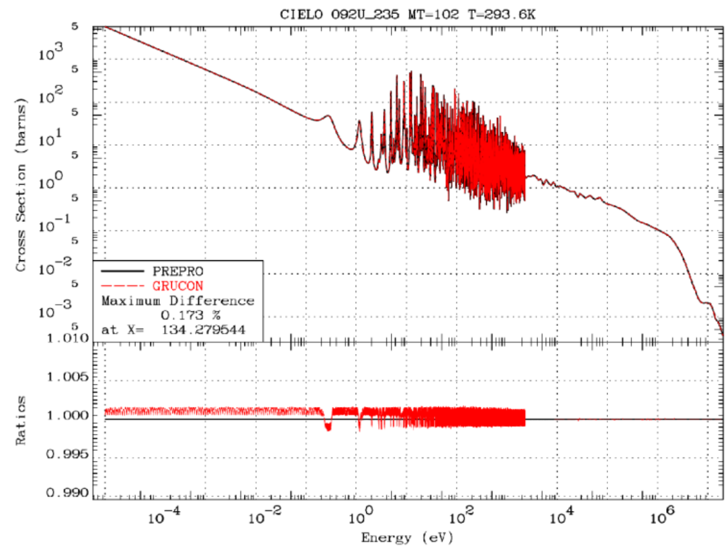
2. Comparison of the Reconstructed from Resonance Parameters and Doppler Broadened Cross Sections

CIELO/ENDF/U-235 : GRUCON/PREPRO comparison

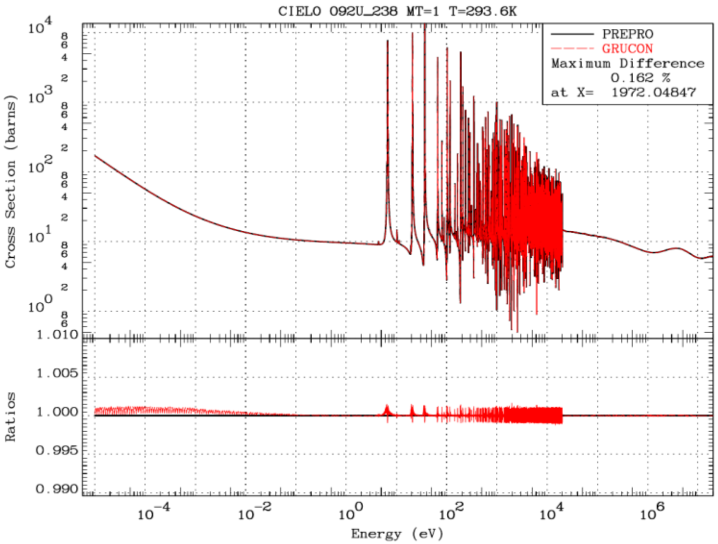


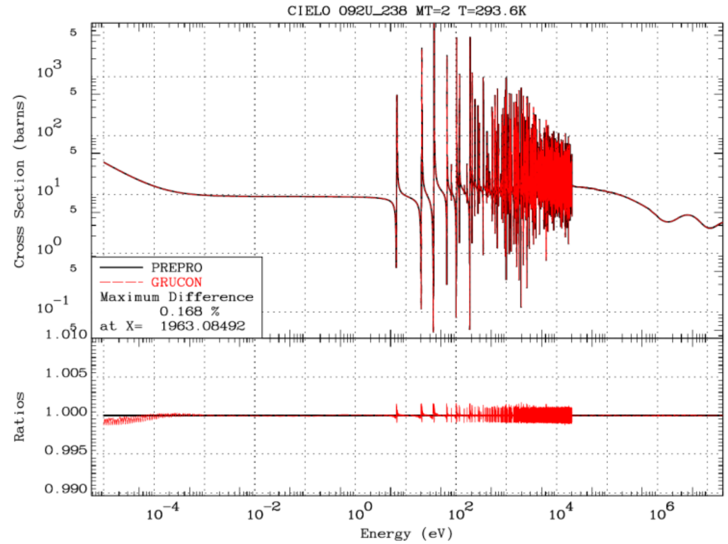


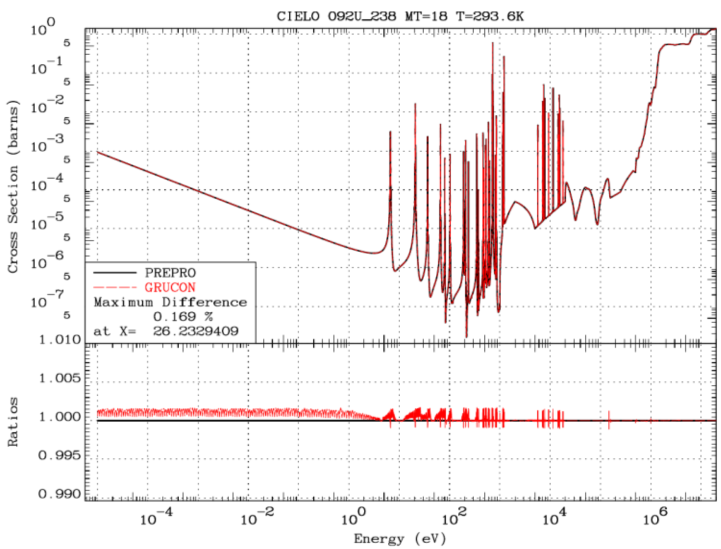


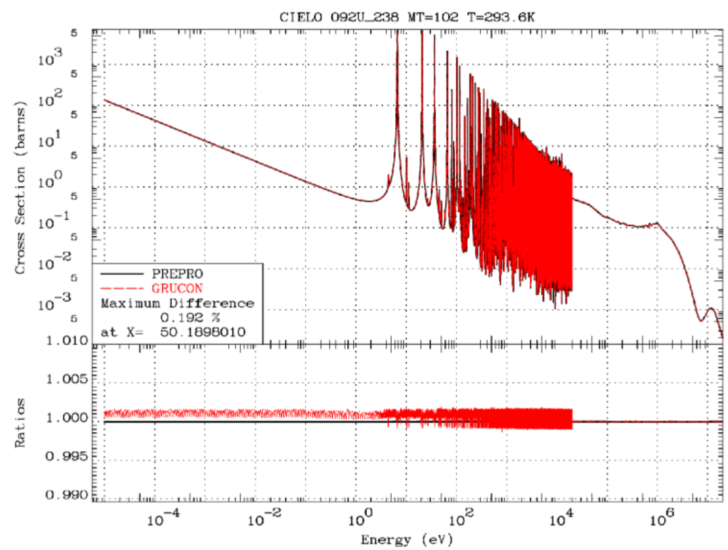


CIELO/ENDF/U-238 : GRUCON/PREPRO comparison

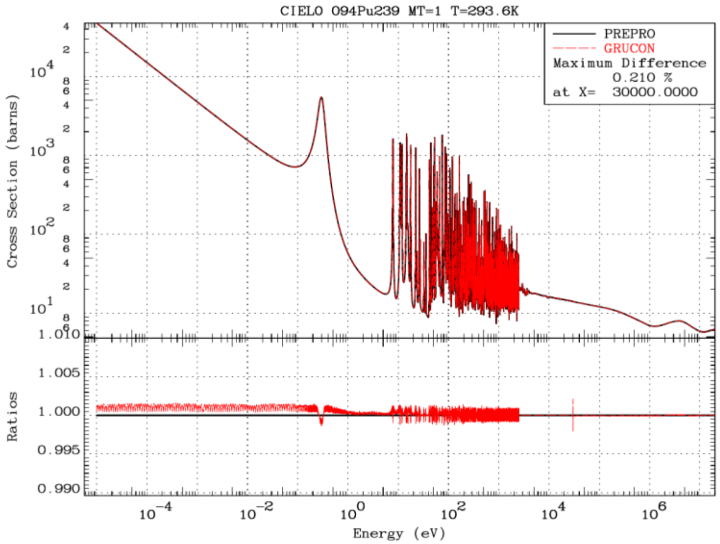


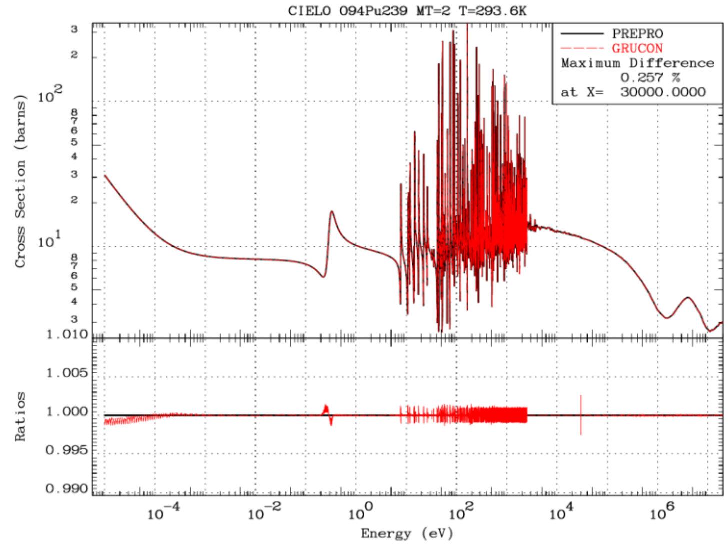


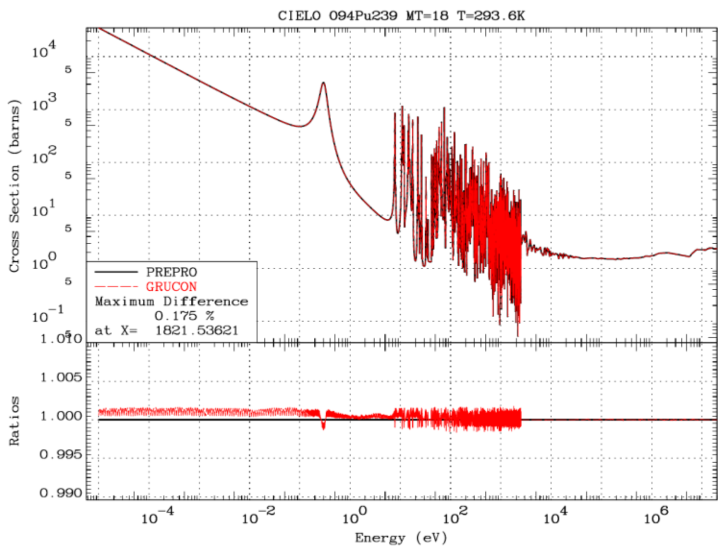


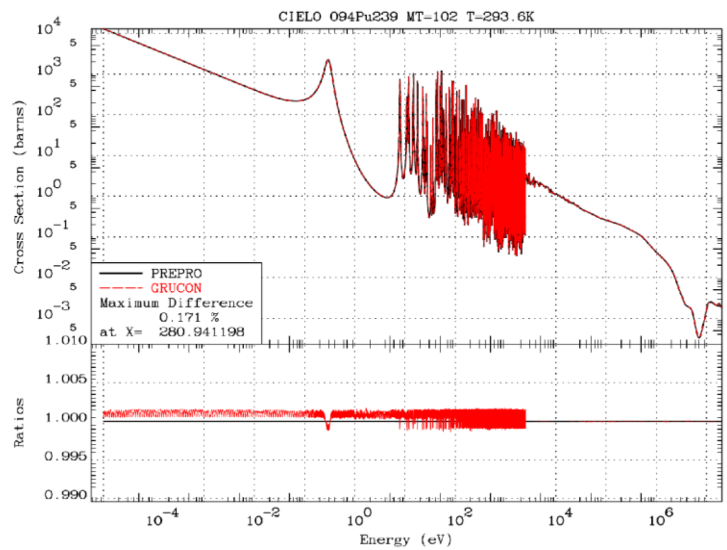


CIELO/ENDF/Pu-239 : GRUCON/PREPRO comparison

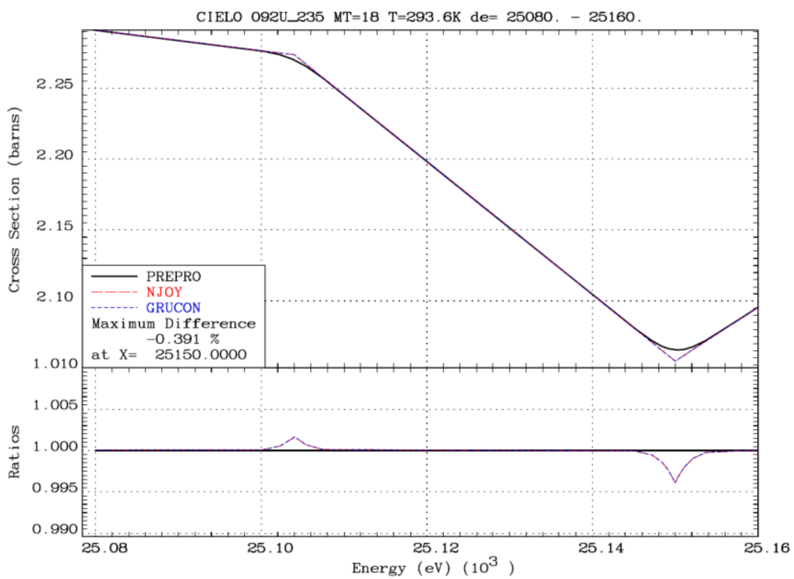


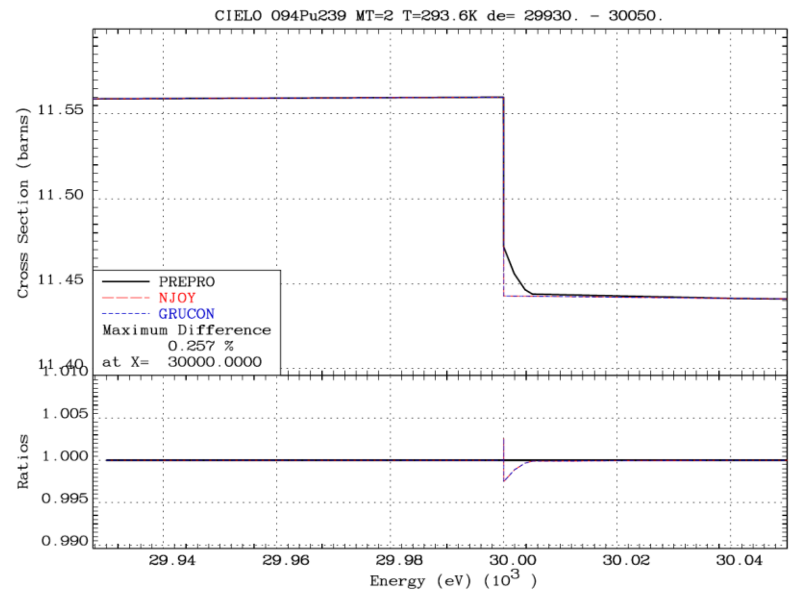




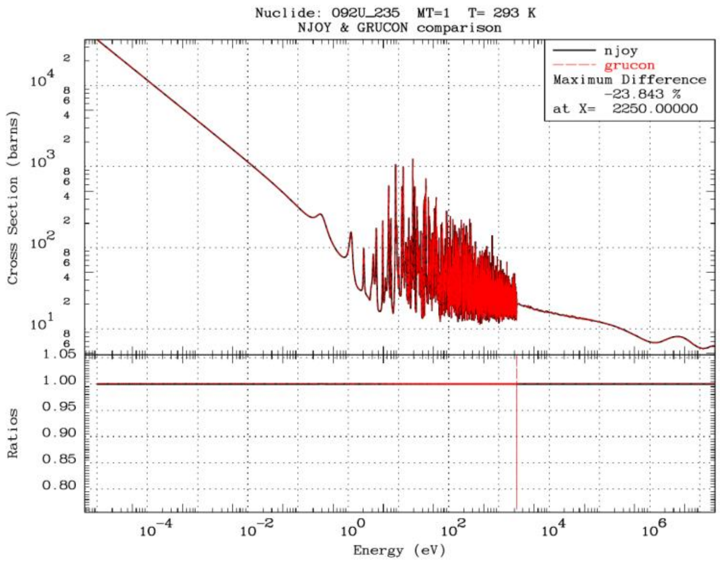


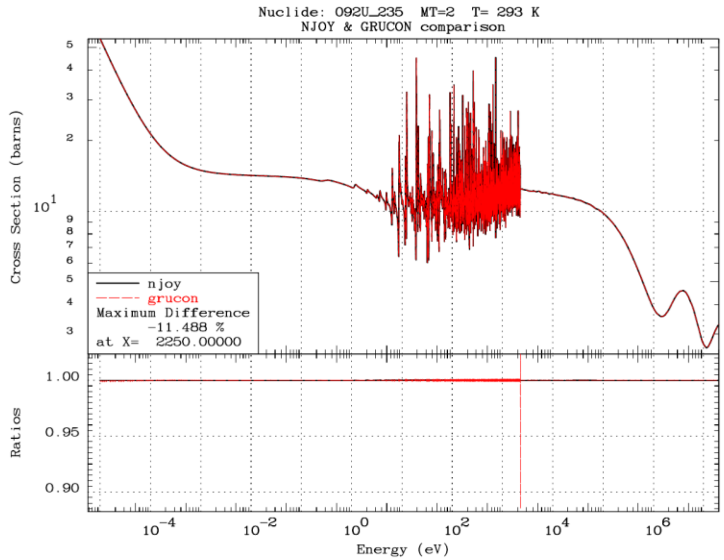
Obtained Difference <0.2% , with exceptions:
U-235 Fission – 0.39%
Pu-239 Elastic – 0.26%
Explanation: GRUCON (and NJOY) don't make Doppler broadening above URR (25keV for U-235 and 30keV for Pu239) , but PREPRO do it:

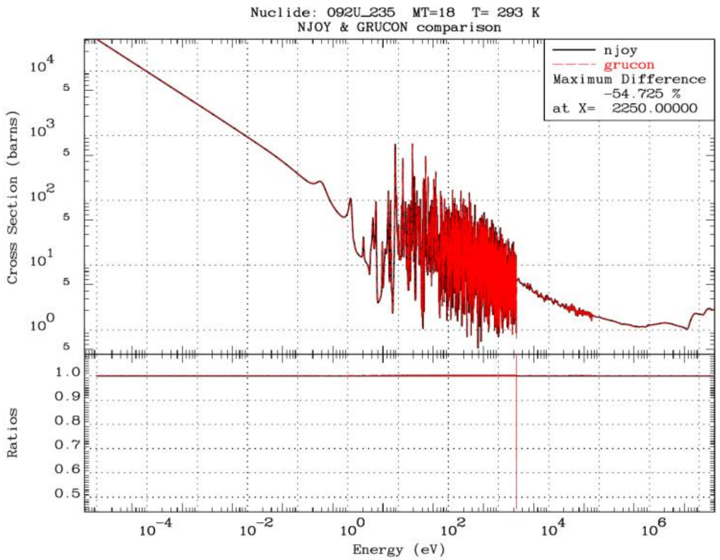


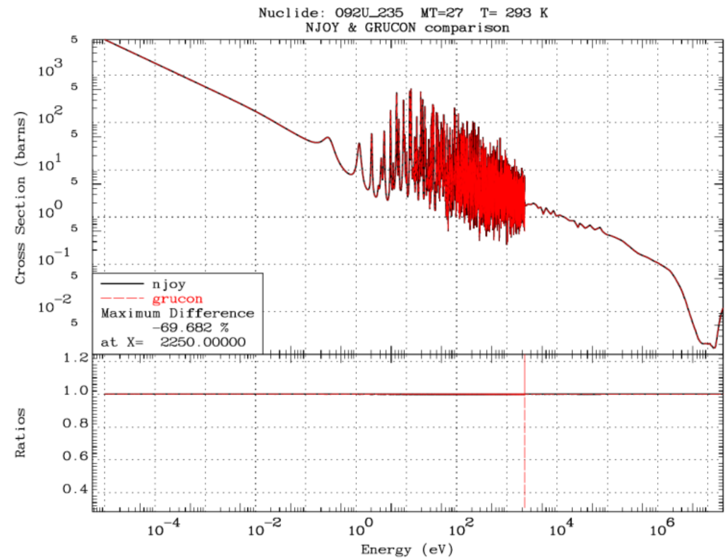


CIELO/ACE/U-235 : GRUCON/NJOY comparison

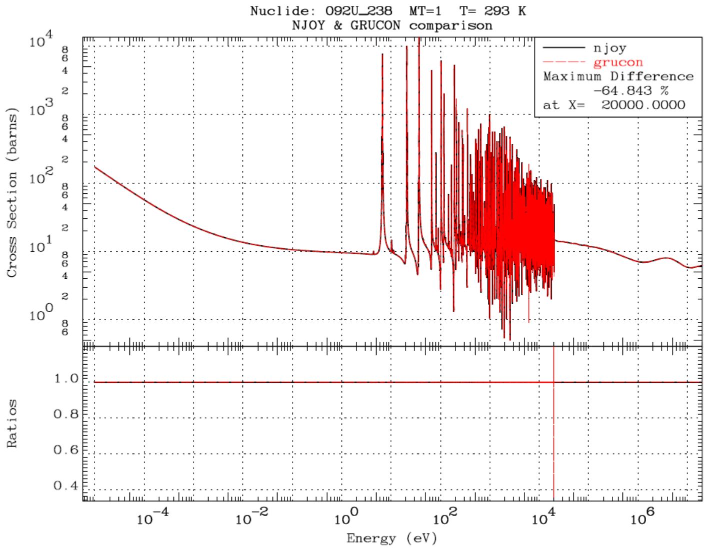


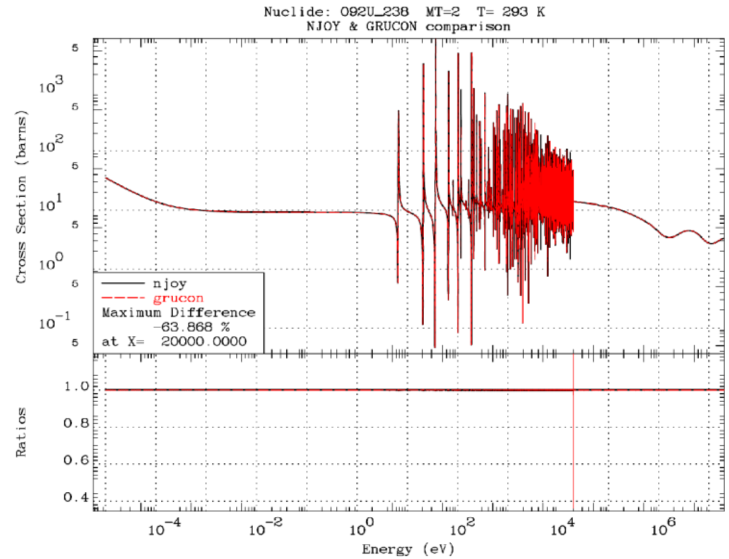


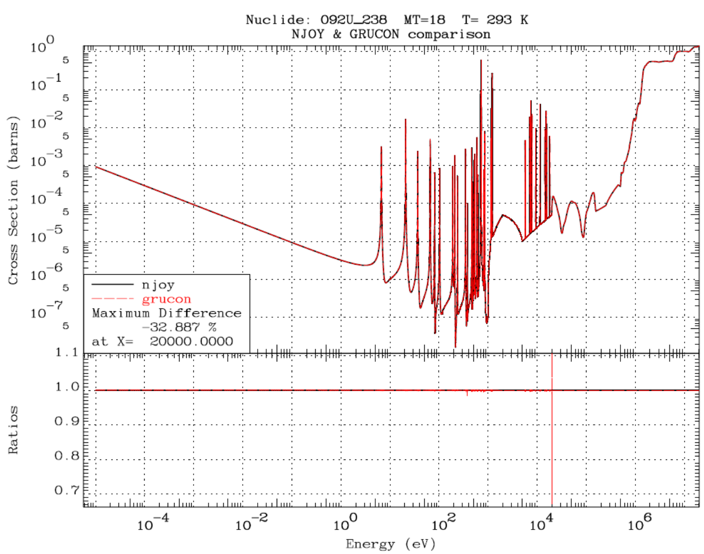


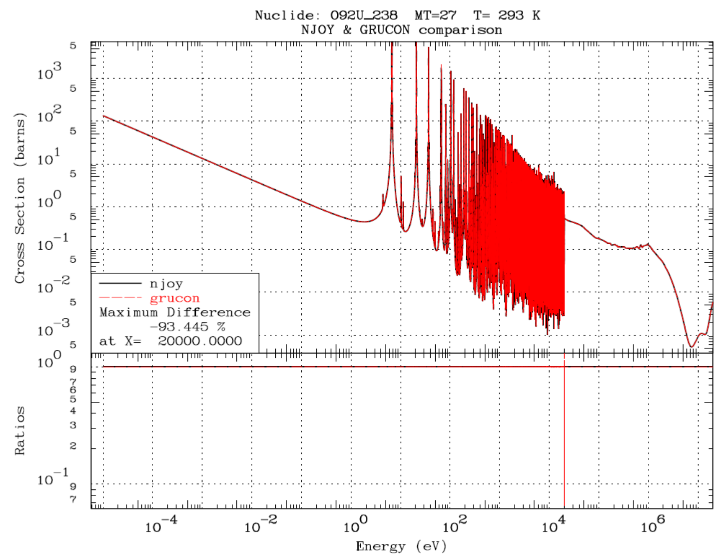


CIELO/ACE/U-238 : GRUCON/NJOY comparison

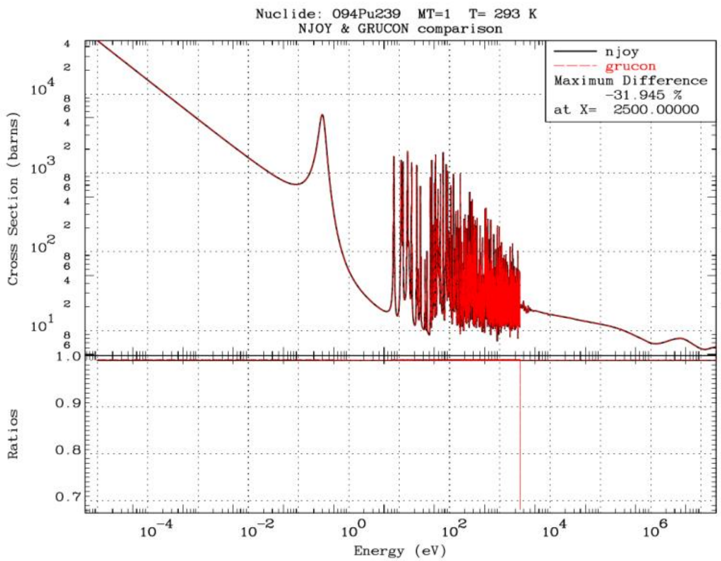


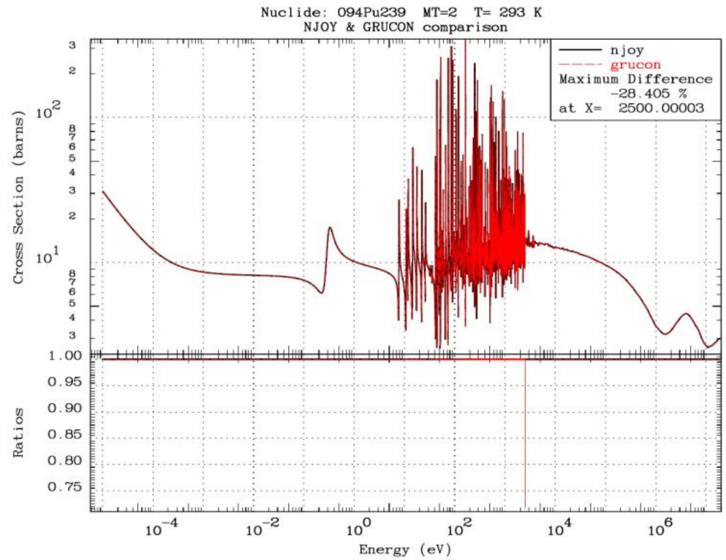


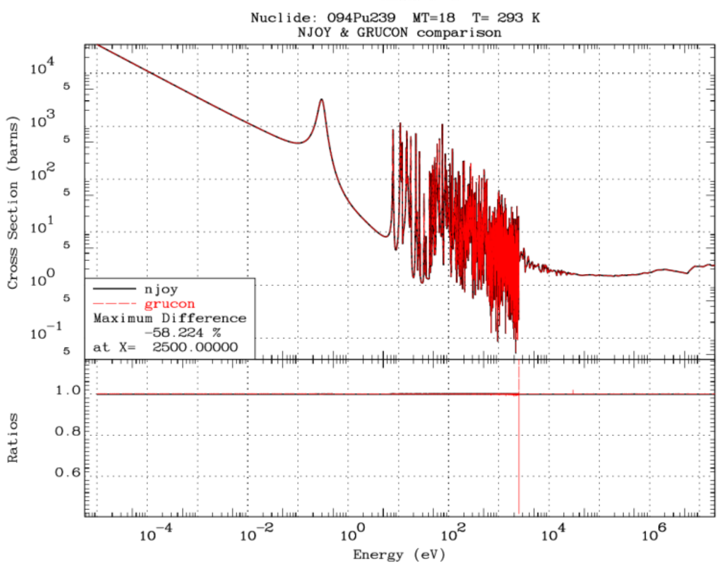


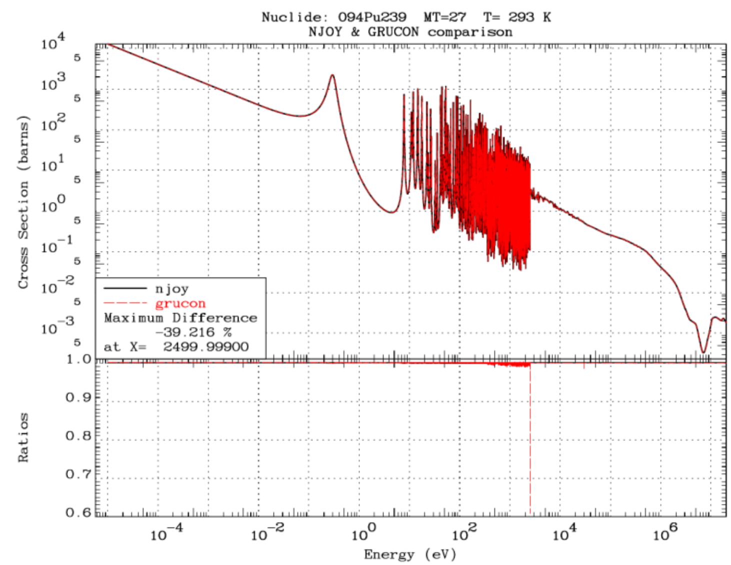


CIELO/ENDF/ACE/Pu-239: GRUCON/NJOY comparison

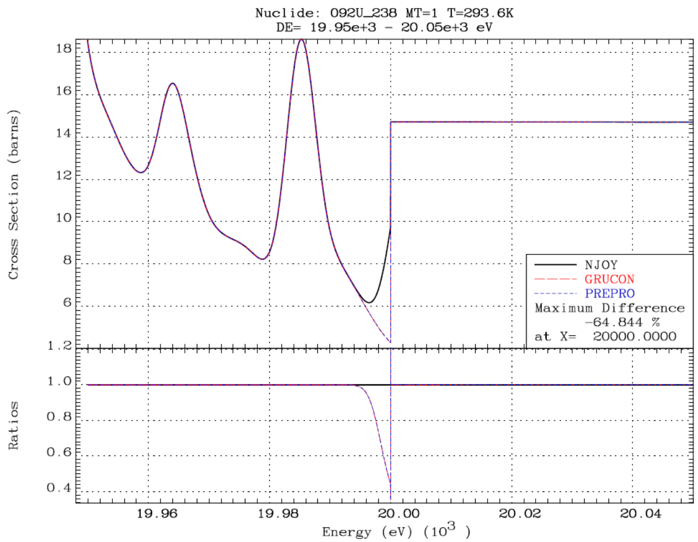


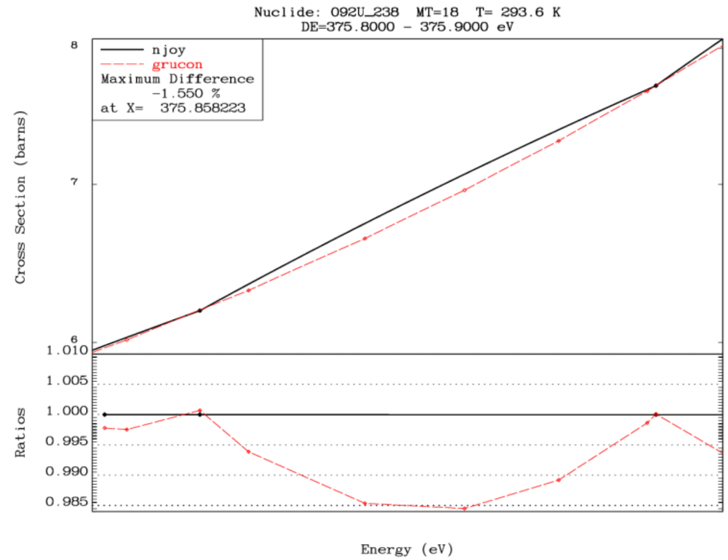


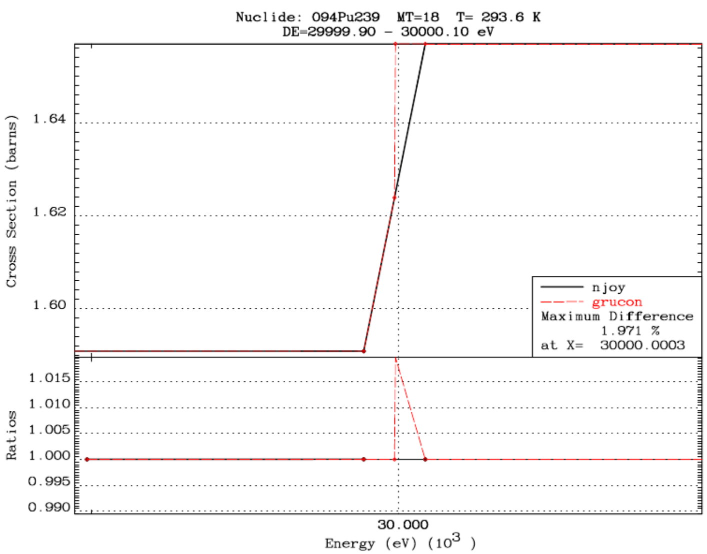


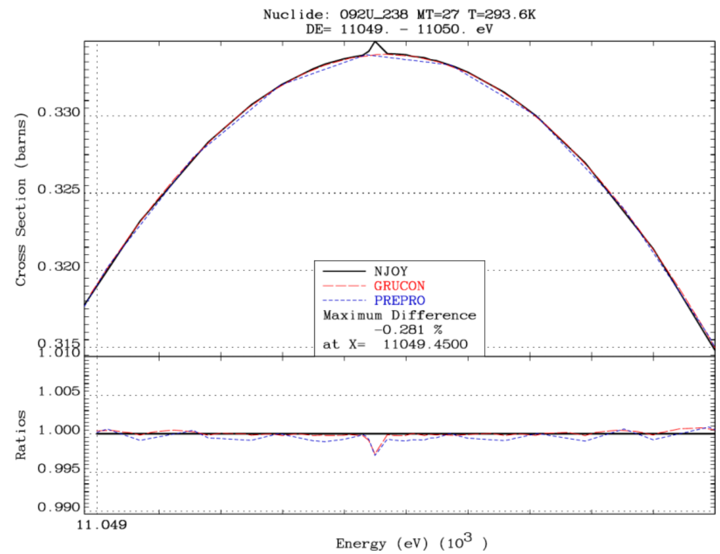


CIELO/ACE/U-238 : some differences









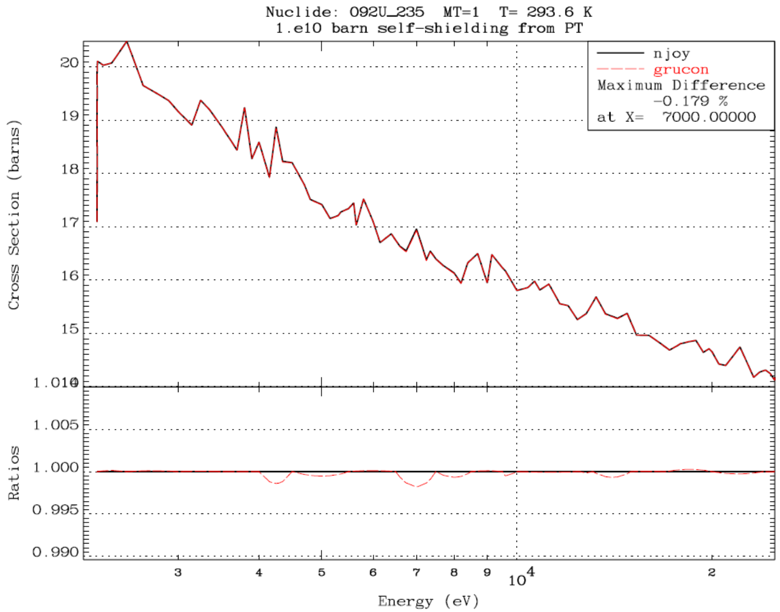
Summary

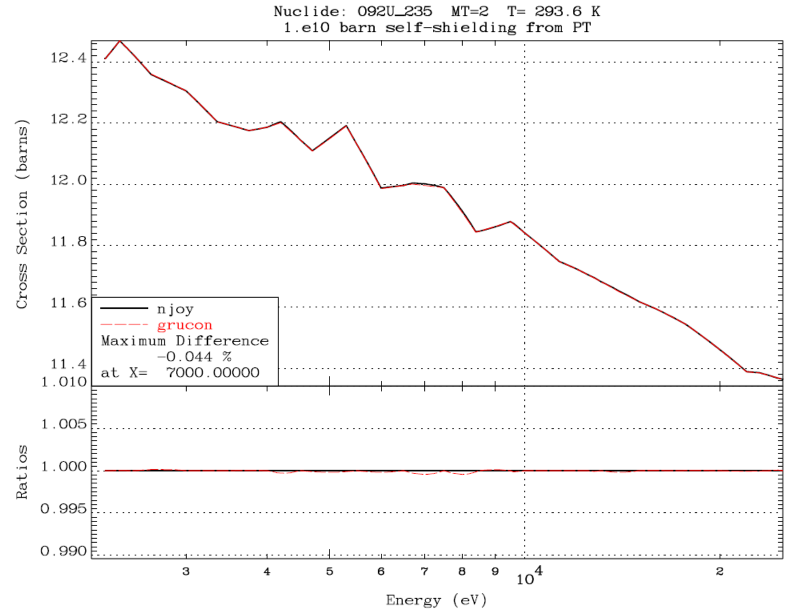
Comparison of cross sections, reconstructed and Doppler broadened through NJOY, PREPRO and GRUCON codes, reveal no serious discrepancies.
ACE files for U-235 and U-238, prepared in CIELO project, sometimes have lack of points in the RR energy range.
The absorption cross section in U238 CIELO ACE file shows irregularity, connected, probably with loss of accuracy.
Differences, found in detailed cross sections, can not have essential influence on results of benchmark calculation.

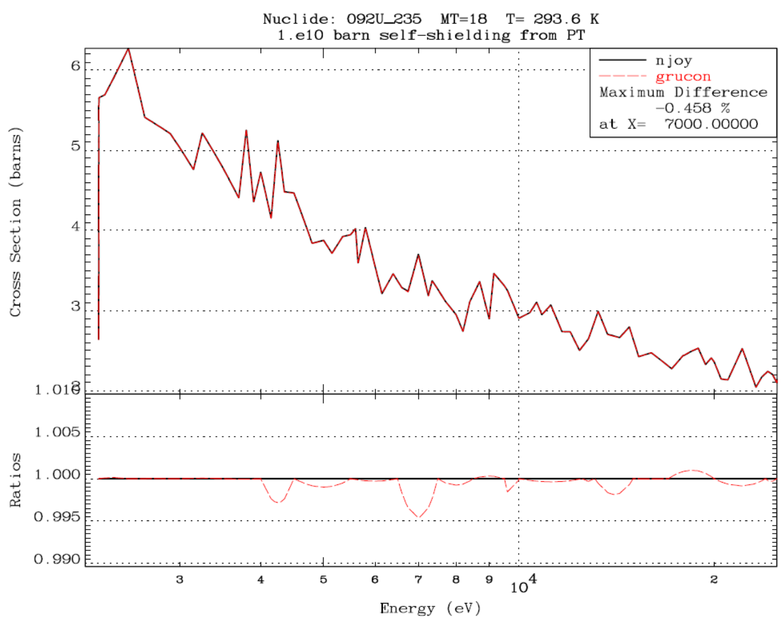
3. Comparison of Cross Sections Derived from Probability Tables and Subgroup Parameters (ACE/LUNR Record)

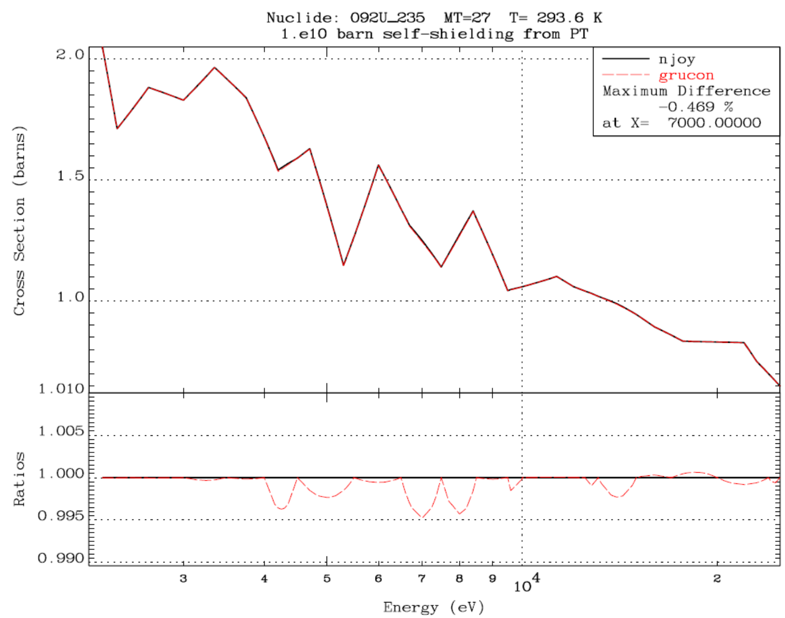
3.1 Comparison of Unshielded Cross Sections Derived from ACE/LUNR Record

CIELO/ACE/U-235: GRUCON/NJOY comparison

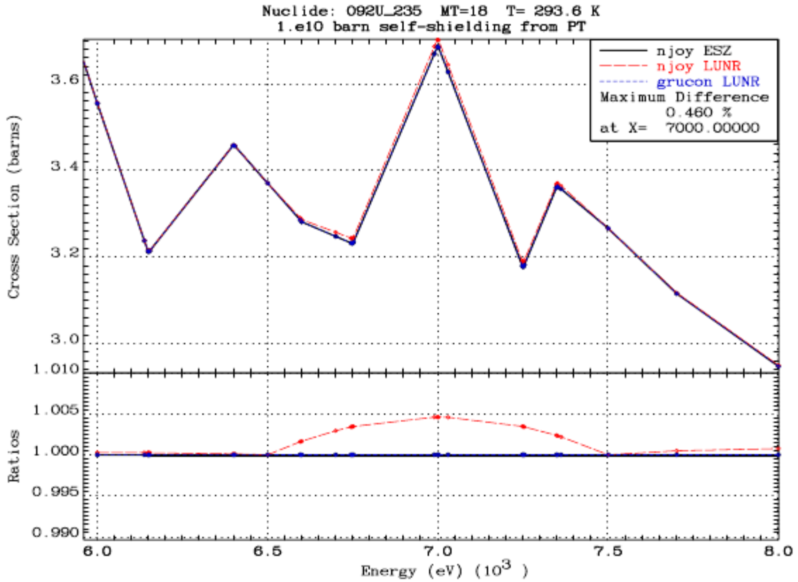


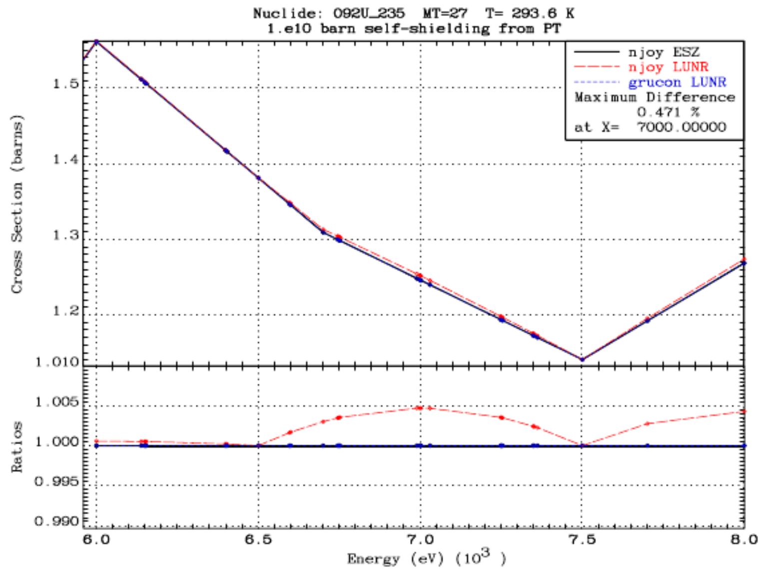




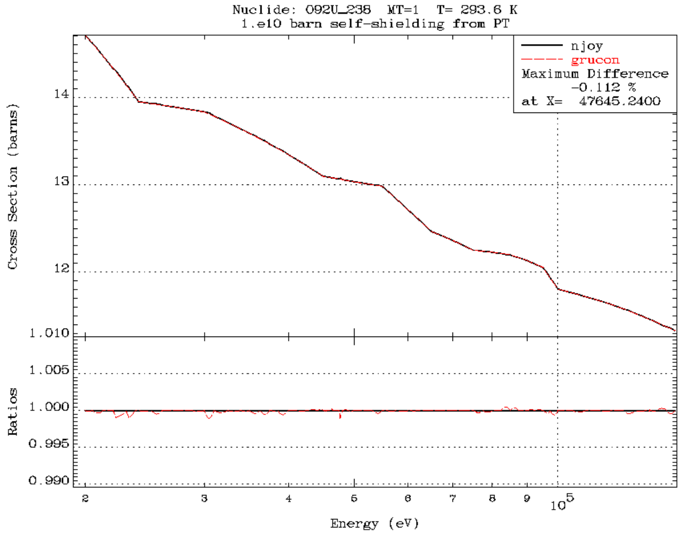


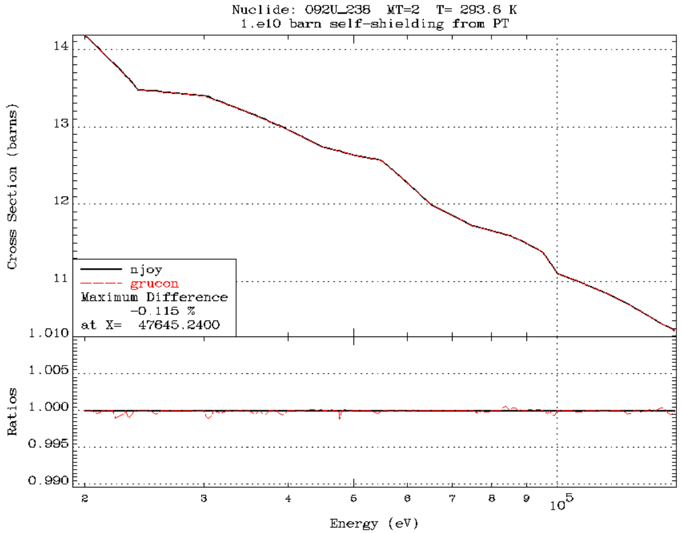
CIELO/ACE/U-235: Comparison of Cross Sections from ACE/ESZ and ACE/LUNR Records

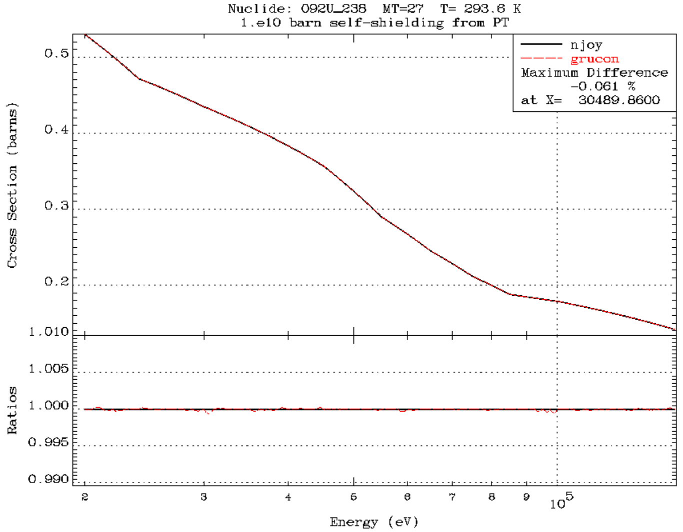




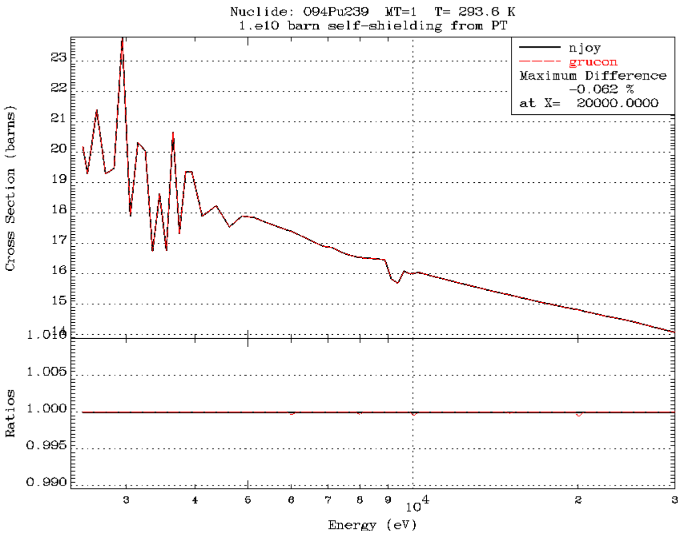
CIELO/ACE/U-238: GRUCON/NJOY comparison

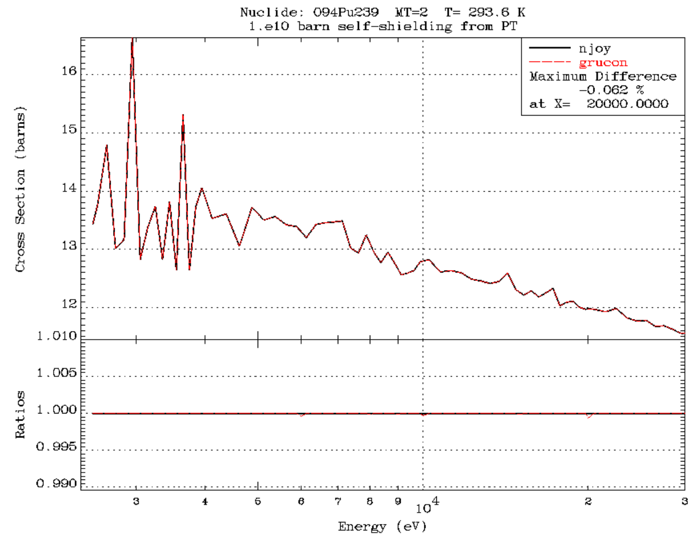


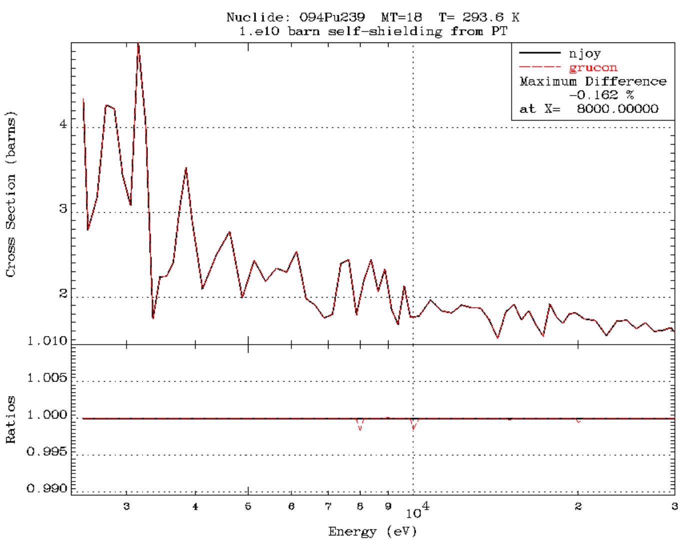


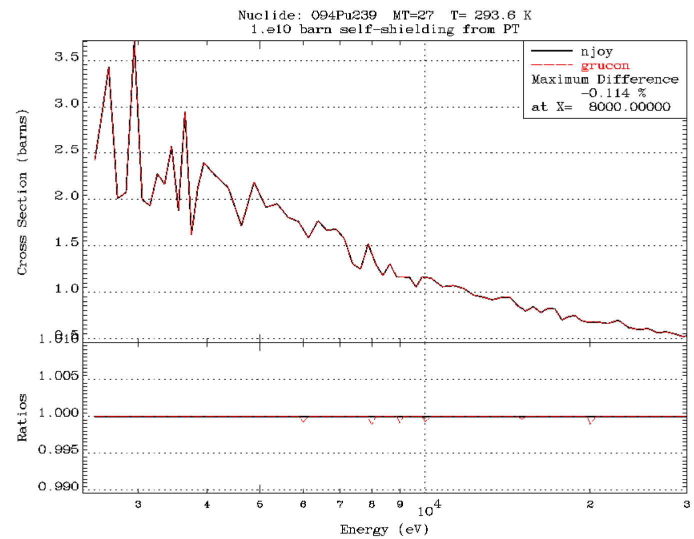


CIELO/ENDF/ACE/Pu-239: GRUCON/NJOY comparison



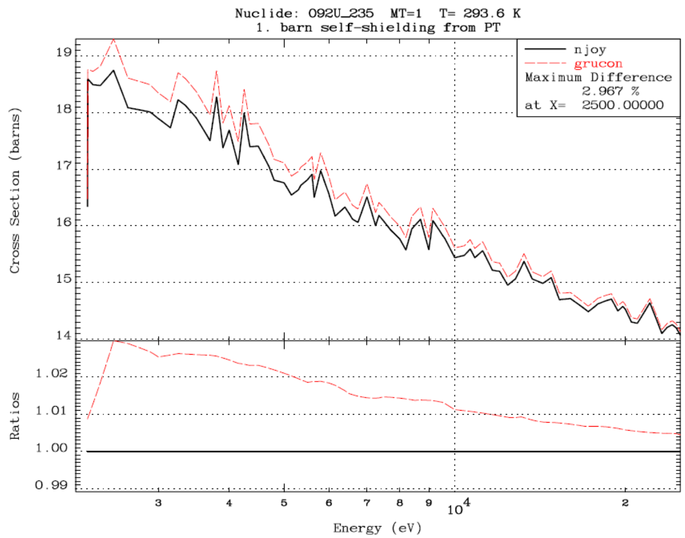


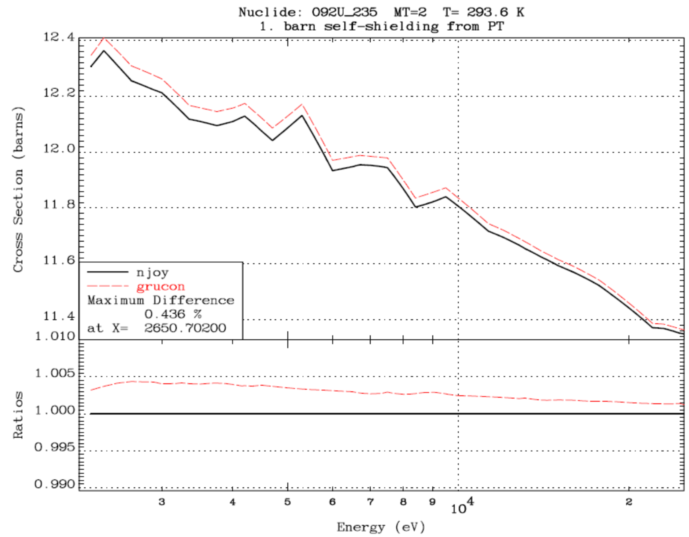


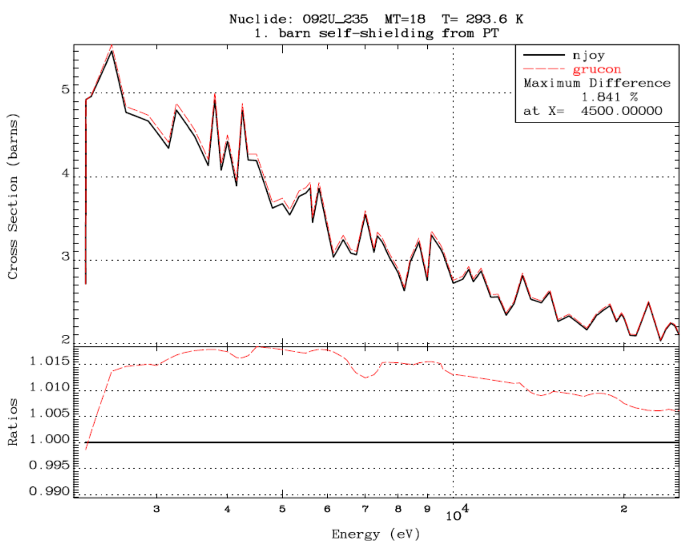


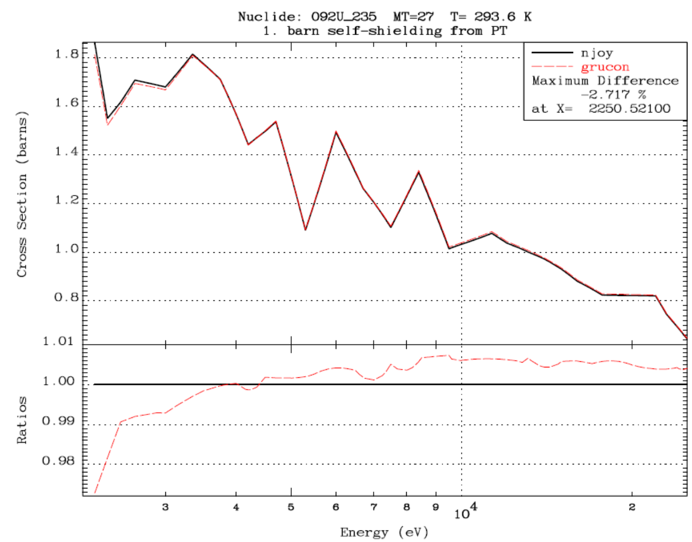
3.2 Comparison of Shielded (1b) Cross Sections Derived from ACE/LUNR Record

CIELO/ACE/U-235: GRUCON/NJOY comparison

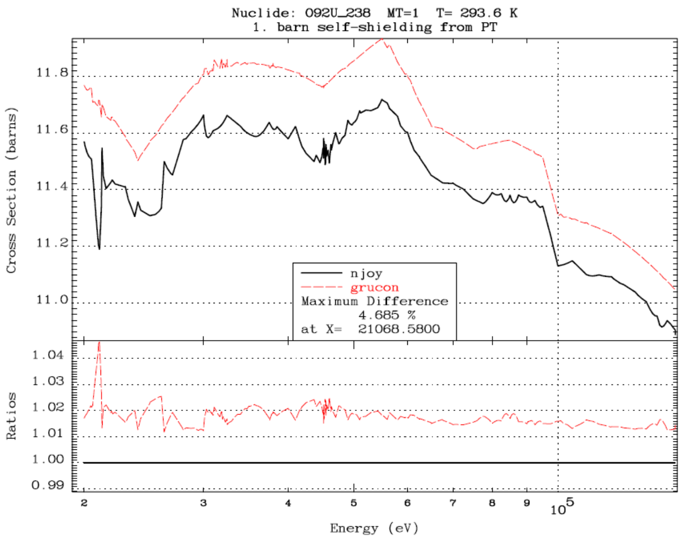


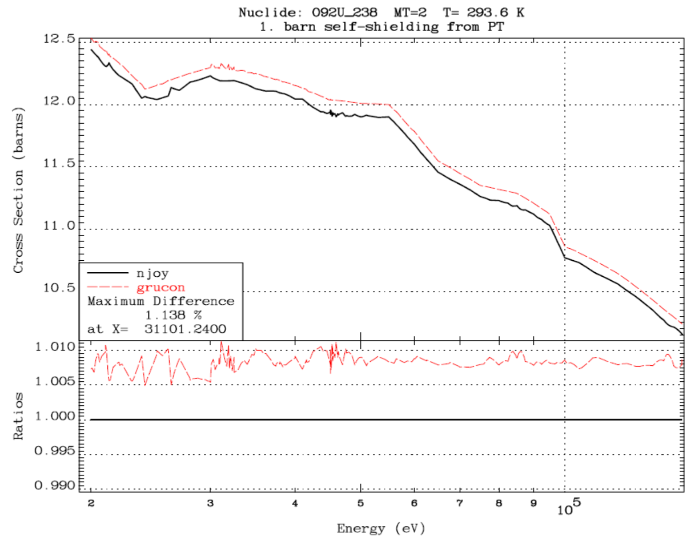


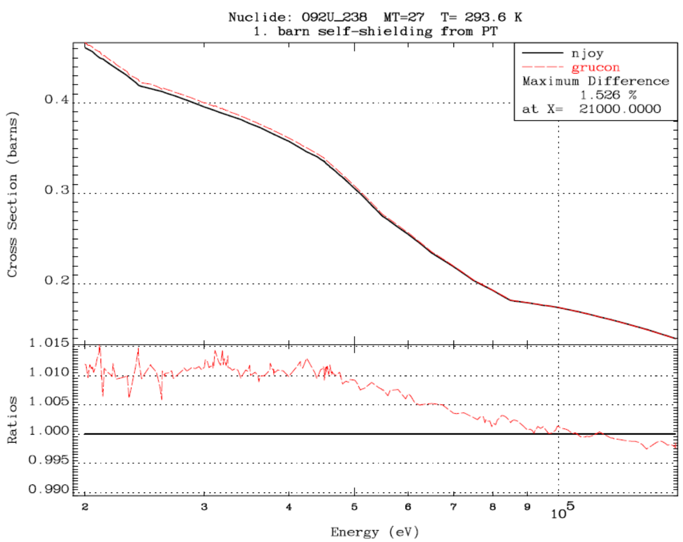




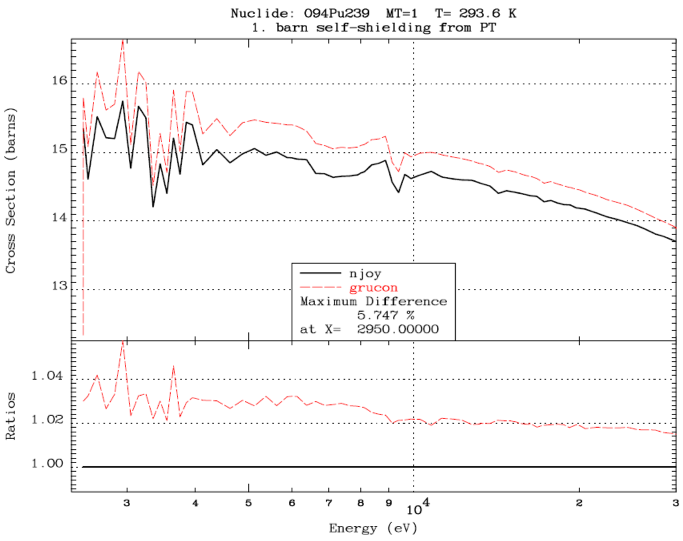
CIELO/ACE/U-238: GRUCON/NJOY comparison

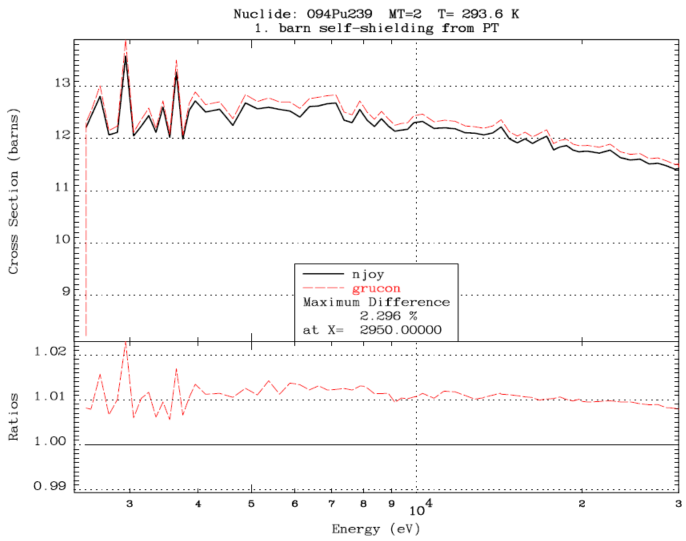


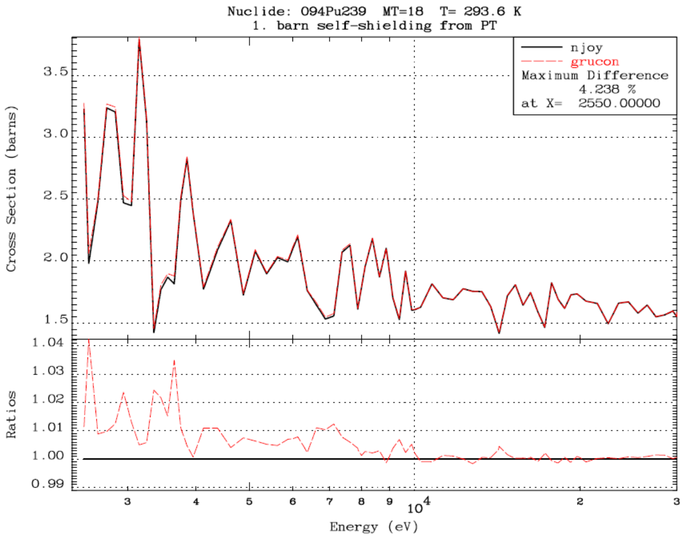


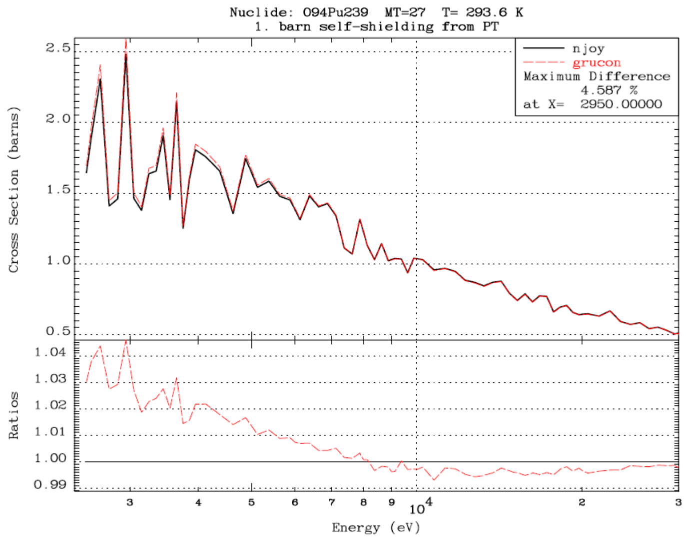


CIELO/ENDF/ACE/Pu-239: GRUCON/NJOY comparison









Summary

Infinitely diluted cross sections, derived from Probability Tables (NJOY) and Subgroup Parameters (GRUCON) reveal no essential disagreement. A small difference (~0.47%), obtained in fission and absorption cross sections of U-235, is due to interpolation error the interpolation error of ACE/LUNR table, prepared by NJOY.

Effective cross sections at 1 barn dilution, in contrary, demonstrate essential differences (up to ~6% in case of total cross section of Pu-239) , and require additional consideration.

4. Keff Calculations

NJOY/MCNP

N	Benchmark	Experiment	Error	Keff (PT)	Error	Keff (NOPT)	Error
0	scherzo -5.56	1.000	0.002	1.00367	0.00005	0.99466	0.00005
1	heu-met-fast-001	1.000	0.001	1.00026	0.00008	1.00012	0.00008
2	heu-met-fast-002	1.000	0.003	0.99988	0.00009	0.99976	0.00009
3	heu-met-fast-003_01	1.000	0.005	0.99322	0.00009	0.99362	0.00009
4	heu-met-fast-003_02	1.000	0.005	0.99239	0.00009	0.99291	0.00009
5	heu-met-fast-003_03	1.000	0.005	0.99718	0.00009	0.99762	0.00009
6	heu-met-fast-003_10	1.000	0.005	1.00453	0.00008	1.00455	0.00009
7	heu-met-fast-003_11	1.000	0.005	1.00923	0.00009	1.00916	0.00010
8	heu-met-fast-014	0.9989	0.0017	0.99549	0.00020	0.99632	0.00009
9	heu-met-fast-032_01	1.0000	0.0016	1.00212	0.00021	1.00282	0.00009
10	heu-met-fast-032_02	1.0000	0.0027	1.00250	0.00020	1.00337	0.00020
11	heu-met-fast-032_03	1.0000	0.0017	0.99837	0.00019	0.99889	0.00020
12	heu-met-fast-032_04	1.0000	0.0017	1.00003	0.00019	1.00029	0.00019
13	ieu-met-fast-007	1.0045	0.0007	1.00397	0.00008	1.00091	0.00007
14	ieu-met-fast-007d	1.0045	0.0007	1.00403	0.00008	1.00102	0.00007
15	ieu-met-fast-10	0.9954	0.0024	0.99575	0.00015	0.99213	0.00015
16	ieu-met-fast-013	0.9941	0.0023	0.99632	0.00016	0.99414	0.00016
17	ieu-met-fast-014-2	0.9958	0.0022	0.99668	0.00016	0.99519	0.00016
18	mix-misc-fast-001_01	0.9736	0.0071	0.96937	0.00012	0.96120	0.00012
19	mix-misc-fast-001_02	1.0050	0.0057	0.99717	0.00013	0.98888	0.00012
20	mix-misc-fast-001_03	0.9959	0.0059	0.98945	0.00014	0.98088	0.00013
21	mix-misc-fast-001_09	1.0188	0.0072	1.01146	0.00014	1.00711	0.00014
22	mix-misc-fast-001_10	0.9732	0.0064	0.97405	0.00013	0.97006	0.00013
23	mix-misc-fast-001_11	1.0153	0.0074	1.01514	0.00015	1.01368	0.00015
24	ieu-met-fast-022_1	1.00077	0.00134	1.00595	0.00008	1.00512	0.00008
25	ieu-met-fast-022_2	0.99325	0.00110	0.99696	0.00009	0.99664	0.00009
26	ieu-met-fast-022_3	0.98748	0.00110	0.98639	0.00011	0.98607	0.00011
27	ieu-met-fast-022_4	0.98629	0.00107	0.99041	0.00011	0.98996	0.00011
28	ieu-met-fast-022_5	0.99775	0.00123	1.00172	0.00011	1.00121	0.00011
29	ieu-met-fast-022_6	1.00121	0.00172	1.00330	0.00010	1.00258	0.00010
30	ieu-met-fast-022_7	0.99758	0.00126	1.00395	0.00011	1.00376	0.00011
31	ieu-met-fast-012	1.00070	0.0027	1.00255	0.00016	1.00030	0.00016
32	ieu-comp-fast-004	0.9978	0.0015	0.99846	0.00017	0.99758	0.00017

GRUCON/MCNP

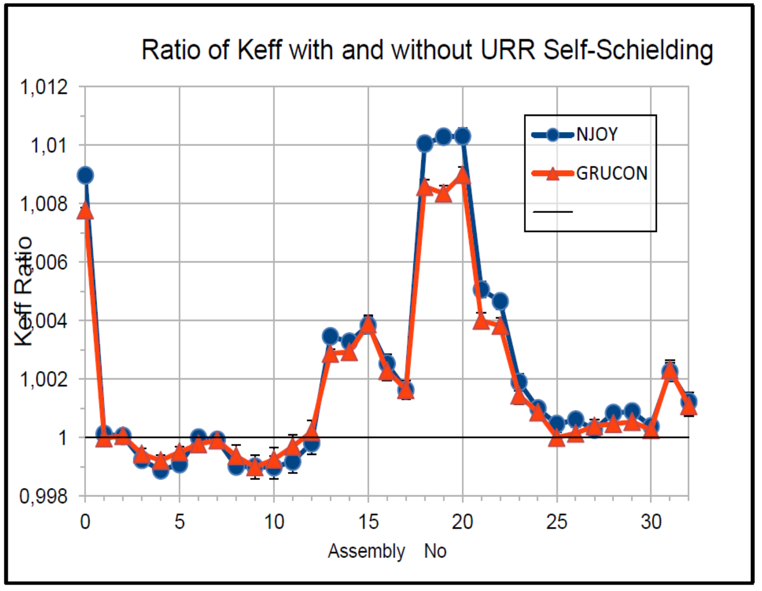
N	Benchmark	Experiment	Error	Keff (SP)	Error	Keff (NOSP)	Error
0	scherzo -5.56	1.000	0.002	1.00240	0.00006	0.99480	0.00005
1	heu-met-fast-001	1.000	0.001	1.00026	0.00008	1.00028	0.00009
2	heu-met-fast-002	1.000	0.003	0.99988	0.00009	0.99982	0.00009
3	heu-met-fast-003_01	1.000	0.005	0.99322	0.00009	0.99378	0.00009
4	heu-met-fast-003_02	1.000	0.005	0.99239	0.00009	0.99317	0.00009
5	heu-met-fast-003_03	1.000	0.005	0.99718	0.00009	0.99767	0.00009
6	heu-met-fast-003_10	1.000	0.005	1.00453	0.00008	1.00475	0.00009
7	heu-met-fast-003_11	1.000	0.005	1.00923	0.00009	1.00932	0.00009
8	heu-met-fast-014	0.9989	0.0017	0.99549	0.0002	0.99612	0.00019
9	heu-met-fast-032_01	1.0000	0.0016	1.00212	0.00021	1.00313	0.0002
10	heu-met-fast-032_02	1.0000	0.0027	1.00232	0.00019	1.00325	0.0002
11	heu-met-fast-032_03	1.0000	0.0017	0.99847	0.0002	0.99867	0.0002
12	heu-met-fast-032_04	1.0000	0.0017	0.99983	0.00019	0.99983	0.00019
13	ieu-met-fast-007	1.0045	0.0007	1.00360	0.00008	1.00109	0.00007
14	ieu-met-fast-007d	1.0045	0.0007	1.00361	0.00008	1.00110	0.00007
15	ieu-met-fast-10	0.9954	0.0024	0.99490	0.00015	0.99190	0.00014
16	ieu-met-fast-013	0.9941	0.0023	0.99600	0.00017	0.99405	0.00016
17	ieu-met-fast-014-2	0.9958	0.0022	0.99661	0.00015	0.99505	0.00015
18	mix-misc-fast-001_01	0.9736	0.0071	0.96932	0.00013	0.96113	0.00012
19	mix-misc-fast-001_02	1.0050	0.0057	0.99735	0.00012	0.98891	0.00012
20	mix-misc-fast-001_03	0.9959	0.0059	0.98925	0.00014	0.98064	0.00014
21	mix-misc-fast-001_09	1.0188	0.0072	1.01146	0.00014	1.00743	0.00013
22	mix-misc-fast-001_10	0.9732	0.0064	0.97394	0.00014	0.97034	0.00013
23	mix-misc-fast-001_11	1.0153	0.0074	1.01512	0.00015	1.01368	0.00015
24	ieu-met-fast-022_1	1.00077	0.00134	1.00575	0.00008	1.00508	0.00008
25	ieu-met-fast-022_2	0.99325	0.00110	0.99637	0.00009	0.99696	0.00009
26	ieu-met-fast-022_3	0.98748	0.00110	0.98582	0.00011	0.98625	0.00011
27	ieu-met-fast-022_4	0.98629	0.00107	0.98971	0.00011	0.99002	0.00011
28	ieu-met-fast-022_5	0.99775	0.00123	1.00122	0.00010	1.00125	0.00011
29	ieu-met-fast-022_6	1.00121	0.00172	1.00206	0.00010	1.00276	0.0001
30	ieu-met-fast-022_7	0.99758	0.00126	1.00328	0.00011	1.00369	0.00011
31	ieu-met-fast-012	1.00070	0.0027	1.00165	0.00016	1.00023	0.00016
32	ieu-comp-fast-004	0.9978	0.0015	0.99796	0.00017	0.99738	0.00018

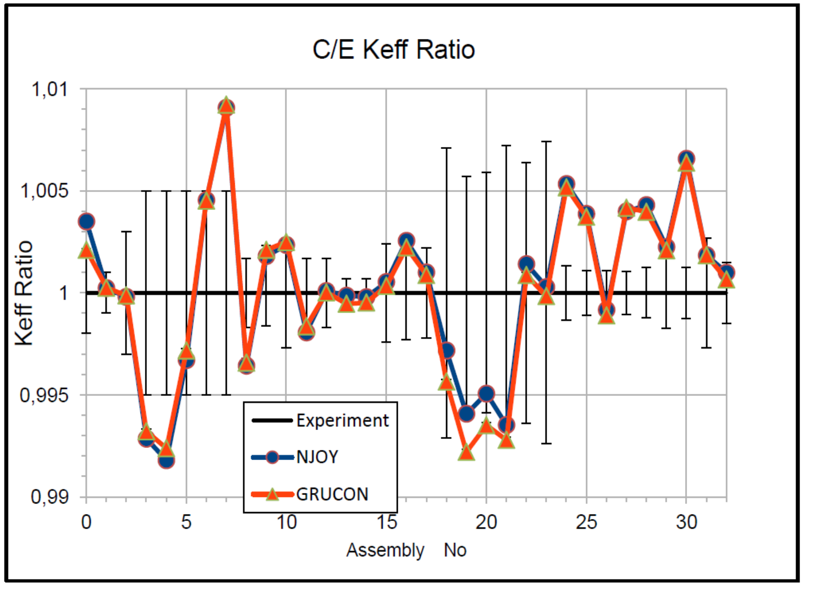
SCHERZO-556 - imaged critical infinity composition of 5.56% ^{235}U and 94.44% ^{238}U.

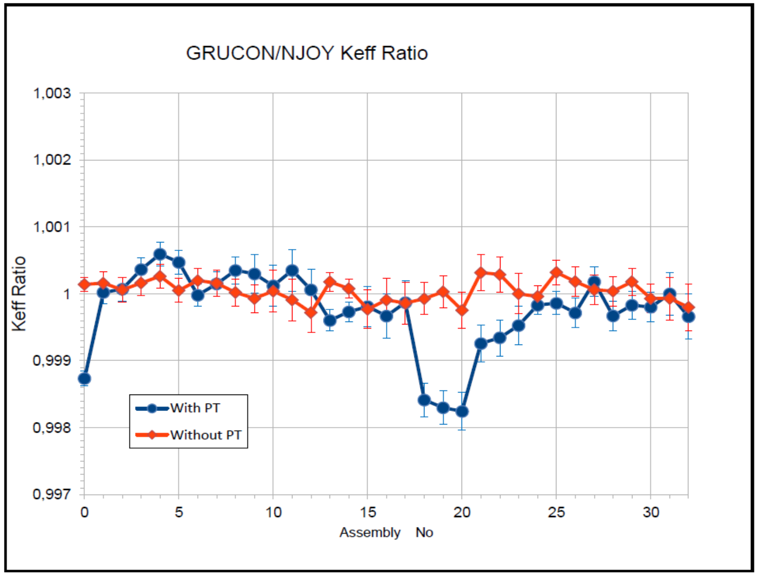
Experiments in Pure Uranium Lattices with Unit Kinf Assemblies SNEAK-8/8Z; UK 1 and UK 5in ERMINE and HARMONIE,
Compiled by *P. Chaudat, M. Darrouzet, E. A. Fischer, Rep.*
KFK 1865, CEA-R-4552 (1974)

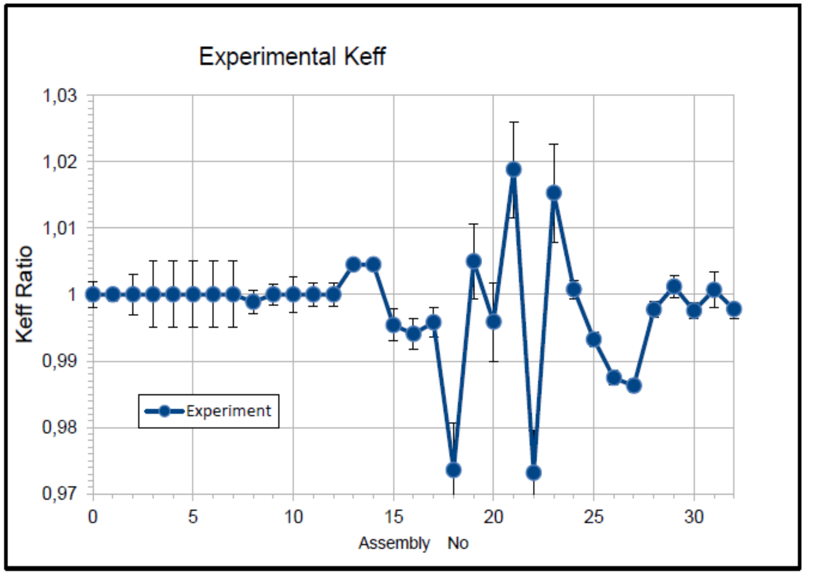
	Experiment	NJOY (PT)	GRUCON (PT)	NJOY (C\E-1)%	GRUCON (C/E-1)%
Kinf	1.000 ± 0.2%	1.00367 (5)	1.00240(6)	0.367	0.240
F238/F235	0.0227 ± 1.3%	0.022122	0.022163	-2.54	-2.37
C238/F235	0.1154 ± 1.5%	0.113749	0.114105	-1.43	-1.12

Comparison of Keff Calculation Results









Summary

Differences in of self-shielded cross sections obtained from Probability Tables {NJOY) and Subgroup Parameters (GRUCON) are manifested in the Keff lowering on ~200 pcm in cases when self-shielding effect in the URR plays an appreciable role (~ 1% in SCERZO-5.56 and MIX-MISC-FAST benchmarks).

Semi-analytical approach to calculation of Cross Section Moments in the URR (U/D-F,U/D-S modules)

Sinitsa V.V., “Calculation of Self-Shielding Factors for Cross Sections in the Unresolved Resonance Region Using the GRUCON Applied Code Package,”
INDC(CCP)-228/GV, Translated by the IAEA, November 1984

Averaging on Resonance Location

Resonance, closest to given E point: $| E_0 - E| \leq \frac{D}{2}$

$$\sigma\ (E, E_0) = \frac{4\pi}{k^2} g \frac{\Gamma_{0n}}{\Gamma_0} \frac{cos2\varphi - \left(2\frac{E_0 - E}{\Gamma_0}\right) sin2\varphi}{1 + \left(2\frac{E_0 - E}{\Gamma_0}\right)^2} + \sigma^B(E, E_0) + \sigma_p$$

$$\sigma_x(E, E_0) = \frac{4\pi}{k^2} g \frac{\Gamma_{0n}\Gamma_{0x}}{\Gamma_0^2} \frac{1}{1 + \left(2\frac{E_0 - E}{\Gamma_0}\right)^2} + \sigma_x^B(E, E_0)$$

Contribution from other resonances:

$$\sigma^B(E, E_0) = \frac{4\pi}{k^2} g \sum_{\lambda \neq 0} \frac{\Gamma_{\lambda n}}{\Gamma_\lambda} \frac{cos2\varphi - \left(2\frac{E_0 - E + \lambda D}{\Gamma_0}\right) sin2\varphi}{1 + \left(2\frac{E_0 - E + \lambda D}{\Gamma_\lambda}\right)^2}$$

$$\sigma_x^B(E, E_0) = \frac{4\pi}{k^2} g \sum_{\lambda \neq 0} \frac{\Gamma_{\lambda n}\Gamma_{\lambda x}}{\Gamma_\lambda^2} \frac{1}{1 + \left(2\frac{E_0 - E + \lambda D}{\Gamma_\lambda}\right)^2}$$

$$\Gamma_\lambda = \sum_x \Gamma_{\lambda x} ;$$

Averaging on Resonance Location (continuation)

Setting $\Gamma_{\lambda,x} = \Gamma_x , \qquad \lambda \neq 0$

and averaging $< (\ldots) > \equiv \frac{1}{D} \int_{E-\frac{D}{2}}^{E+\frac{D}{2}} dE_0 \, (\ldots),$

we finally obtain for contribution of all resonances, except the closest one (with λ=0)

$$< \sigma^B \, (E) >= \frac{4\pi}{k^2} g \frac{\Gamma_n}{D} \left(\frac{\pi}{2} - arctg \frac{D}{\Gamma} \right) cos2 \, \varphi$$

$$< \sigma_x^B \, (E) >= \frac{4\pi}{k^2} g \frac{\Gamma_n \Gamma_x}{\Gamma D} \left(\frac{\pi}{2} - arctg \frac{D}{\Gamma} \right)$$

Averaging on Parameter Distributions

For any x -reaction: $$\sigma_x \sim \frac{\Gamma_n \Gamma_x}{(\Gamma_n+\Gamma_x+\cdots+\Gamma_z)^2} \sim \frac{x}{(x+\gamma)^2}$$

where $x = \frac{\Gamma_x}{\overline{\Gamma}_x}$, and γ includes all other reaction widths: $\gamma = \frac{1}{\overline{\Gamma}_x}\sum_{y\neq x}\Gamma_y$

If x is distributed as

$$P_\nu(x) = \frac{\nu}{2\Gamma(\frac{\nu}{2})}\,(\frac{x\nu}{2})^{\frac{\nu}{2}-1} e^{-\frac{x\nu}{2}}$$

the M_n moments can be axpressed as

$$M_n = \int_0^\infty (x+\gamma)^n\, P(x)dx = \gamma^n \left(\frac{\gamma\nu}{2}\right)^{\frac{\nu}{2}} U(\frac{\nu}{2}, \frac{\nu}{2}+n+1; \frac{\gamma\nu}{2})$$

where *U(a,b; z)* - hyper geometrical function, defined from recurrent relation:

$$(b-a-1)U(a,b-1;z) + (1-b-z)U(a,b;z) + zU(a,b+1;z) = 0$$

with initial values: $U(a,a+1;z) = z^{-a}$

$U(a,a;z) = e^z\,\Gamma(1-a,z)$

Setting $\overline{\gamma}_x = \frac{1}{\overline{\Gamma}_x}\sum_{y\neq x}\overline{\Gamma}_y$, the set of quadrature parameters $\{a_i, x_i\}_{i=1}^{i=N}$

for x -reaction can be found as solution of equation

$$M_n = \sum_{i=1}^{i=2N} a_i\,(x_i+\overline{\gamma}_x)^n, \qquad L - N \le n \le L+N-1$$

Averaging on Parameter Distributions (continuation)

The moments for each spin group , averaged on parameter distributions, are summation by quadrature formulas

$$\overline{< M_n \ (\sigma_x(E;T), \sigma(E;T)) >} \cong \sum_{i_1}^{N_1} \dots \sum_{i_m}^{N_m} a_{i_1} \times \ \dots \times a_{i_m} < M_n \left(\sigma_x \ (E;T), \sigma(E;T) | \ x_{i_1}, \dots, x_{i_m}\right) >$$

of the moments, averaged numerically on resonance location

$$< M(\sigma_x(E;T), \sigma(E;T) | \ x_1, \dots, x_m) > = \frac{1}{D} \int_{E-\frac{D}{2}}^{E+\frac{D}{2}} dE_0 < M(\sigma_x(E, E_0;T), \sigma(E, E_0;T) | \ x_1, \dots, x_m) >$$

for cross sections, defined by formulas

$$\sigma \ (E, E_0;T) = \frac{4\pi}{k^2} g \frac{\Gamma_{0n}}{\Gamma_0} (\Psi \ (x, \xi) cos2\varphi + \mathrm{X}(x, \xi) sin2\varphi) + \overline{< \sigma^B \ (E) >} + \ \sigma_p$$

$$\sigma_x(E, E_0;T) = \frac{4\pi}{k^2} g \frac{\Gamma_{0n}\Gamma_{0x}}{\Gamma_0^2} \Psi \ (x, \xi) + \overline{< \sigma_x^B \ (E) >}$$

$$x = 2 \frac{E - E_0}{\Gamma_0}; \qquad \xi = \frac{\Gamma_0}{\Delta}; \qquad \Delta = 2 \sqrt{\frac{k_B T E}{M/m_n}}$$

Moments convolution (F/C-F module)

Badikov S.A., Gai E.V., Rabotnov N.S.,Sinitsa V.V.,
“Use of Padé Approximation to calculate subgroup constants and to Include the Doppler Effect in Resonance Analysis of Neutron Cross Sections,”
Soviet Atomic Energy, Volume 60, Issue 1 (1986) pp 35-43

Rineiski A.A., Sinitsa V.V.,
“Extended Probability Tables for Approximation Multigroup Cross –Sections,”
M&C, Gatlinburg, Tennessee, April 6-11,2003

Type of Moments

Rational Moments (shielded cross sections)	Exponential Moments (transmission functions)
$S_n\,(\sigma\,|\sigma_0) = \overline{<(\sigma+\sigma_0)^n>}$	$T_n\,(\sigma\,|\,t_0) = \overline{<e^{-\sigma t_0 n}>}$
$S_n(\sigma_x, \sigma\,|\,\sigma_0) = \overline{<\sigma_x\,(\sigma+\sigma_0)^n>}$	$T_n(\sigma_x\,, \sigma|\,t_0) = \overline{<\sigma_x\,e^{-\sigma t_0 n}>}$

	Allowable moment's parameters:		**Approximations:**
(a)	σ_0 = const,	L - N ≤ n ≤ L+N-1	(*Gauss*)
(b)	n = -1 (fixed),	set of values $\{\sigma_{0j}\}_{j=1}^{j=M}$	(*Padé-II*)
(c)	t_0 = const,	0 ≤ n ≤ 2N-1	(Gauss)
(d)	n = 1 (fixed)	$\{t_{0i}\}_{i=1}^{M}$	(no approximation)

Rational Moment Approximations

Gauss quadrature approach

$\sigma_0 = const\,, \qquad L - N \le n \le L + N - 1$

$$< (\sigma + \sigma_0)^n > = \sum_{i=1}^{N} a_i\,(\sigma_i + \sigma_0)^n$$

$$< \sigma_x(\sigma + \sigma_0)^n > = \sum_{i=1}^{N} (a\sigma_x)_i \left(\sigma_i^{(x)} + \sigma_0\right)^n$$

Padé-II **approximation approach**

$n = -1\ (fixed) \qquad \{\sigma_{0j}\}_{j=1}^{j=M \ge 2N}$

$$< 1/(\sigma + \sigma_{0j}) > \cong \sum_{i=1}^{N} a_i\,/(\sigma_i + \sigma_{0j})$$

$$< \frac{\sigma_x}{\sigma + \sigma_{0j}} > \cong \sum_{i=1}^{N} (a\sigma_x)_i\,/(\sigma_i^{(x)} + \sigma_{0j})$$

Rational Moments Convolution

$$S_n\,(\,\sigma|\sigma_0) = \sum_{\vec{i}} a_{\vec{i}}\; S_n(\sigma_{\vec{i}}|\sigma_0) \quad ; \quad a_{\vec{i}} \equiv \prod_{m=1}^{M} a_{i_m}$$

$$\sigma_{\vec{i}} \equiv \sum\nolimits_{m=1}^{M} \sigma_{i_m}$$

M – number of components

$$\vec{i} \equiv (i_1, i_2, \ldots\; i_M)$$

$$i_m = 1, \;\ldots\;,\; N_m$$

$$S_n\,(\,\sigma_x, \sigma|\sigma_0) = \sum\nolimits_{m=1}^{M} \sum_{\vec{i}} a_{\vec{i}}^{(m)} S_n\left(\sigma_{\vec{i}}^{(m)}\middle|\sigma_0\right) \quad ; \quad a_{\vec{i}}^{(m)} \equiv (a\sigma_x)_{i_m} \prod_{k\neq m} a_{i_k}$$

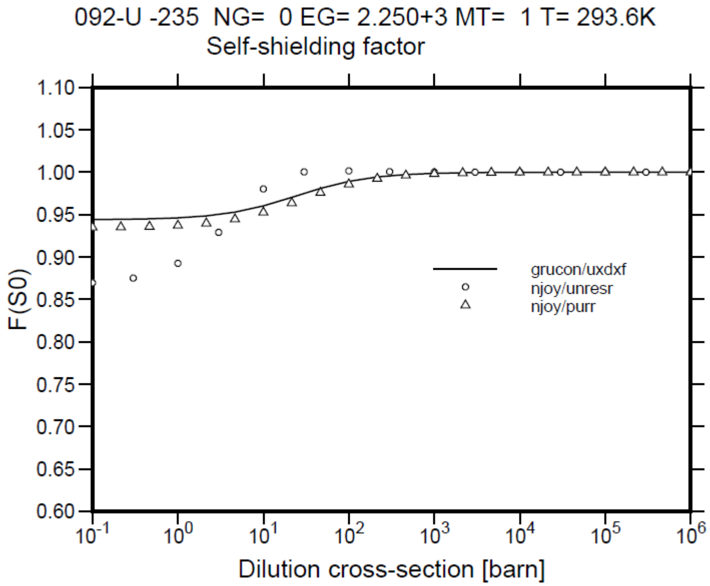
$$\sigma_{\vec{i}}^{(m)} \equiv \sigma_{i_m}^{(x)} + \sum_{k\neq m} \sigma_{i_k}$$

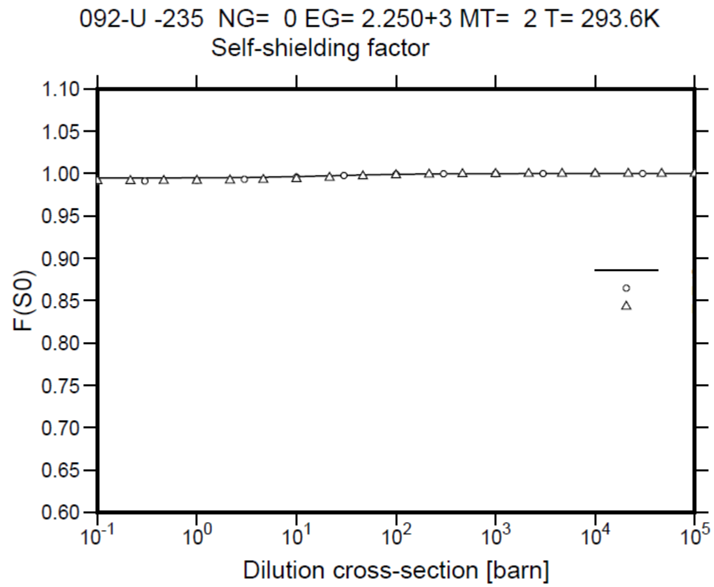
Exponential Moments Convolution

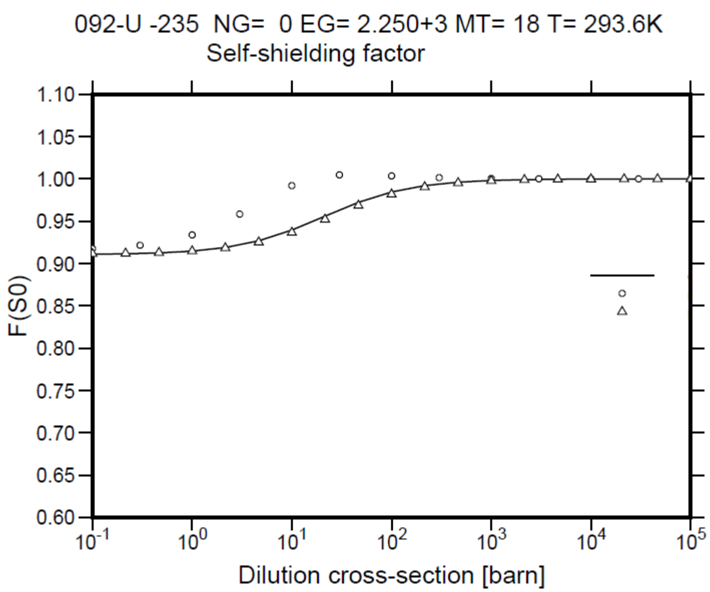
$$T_n(\sigma|t) = \prod_{m=1}^{M} T_n(\sigma^{(m)}|t)$$

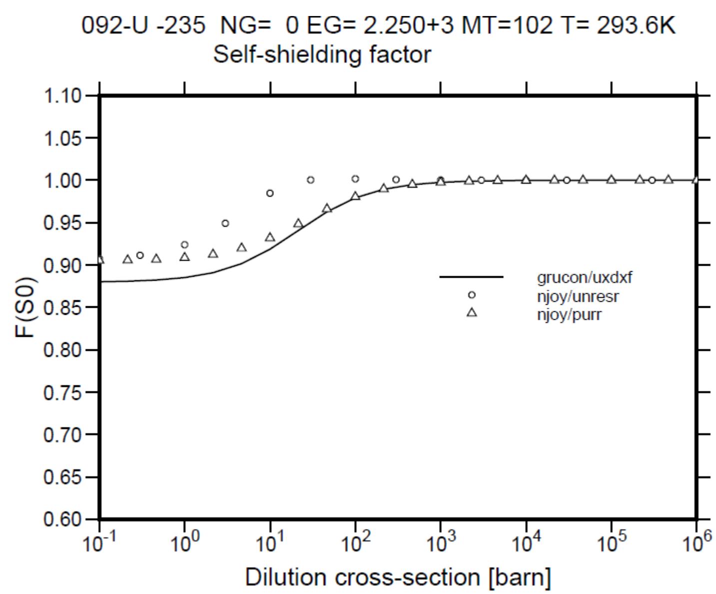
$$T_n(\sigma_x, \sigma|t) = \sum_{m=1}^{M} \left\{ T_n(\sigma_x^{(m)}, \sigma^{(m)}|t) \prod_{k\neq m} T_n\,(\sigma^{(k)}|t) \right\}$$

U-235 URR SS Factors: GRUCON/NJOY comparison

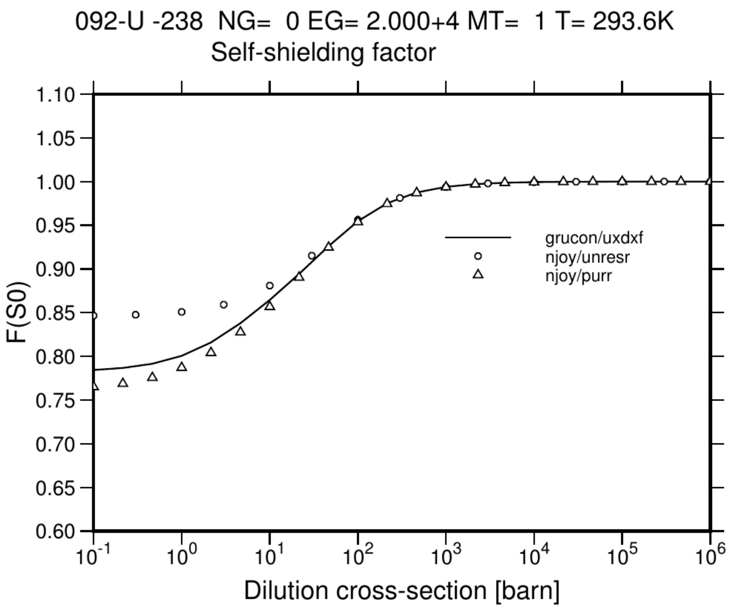


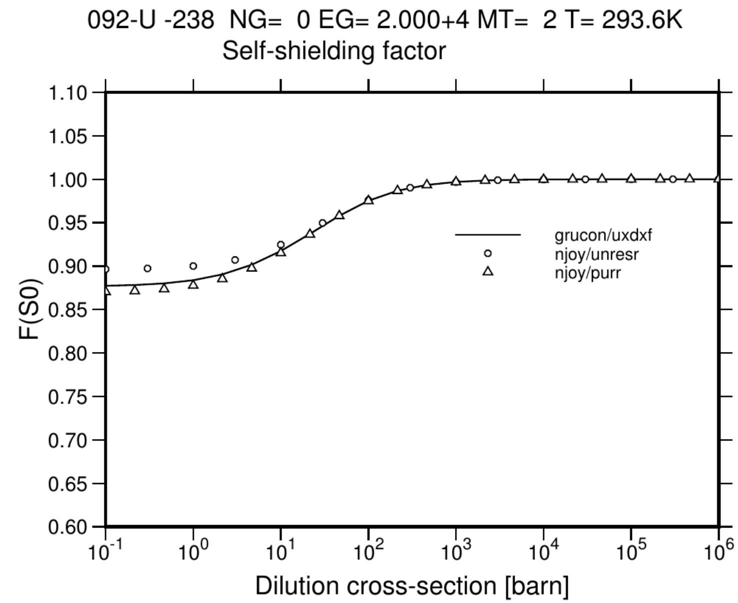


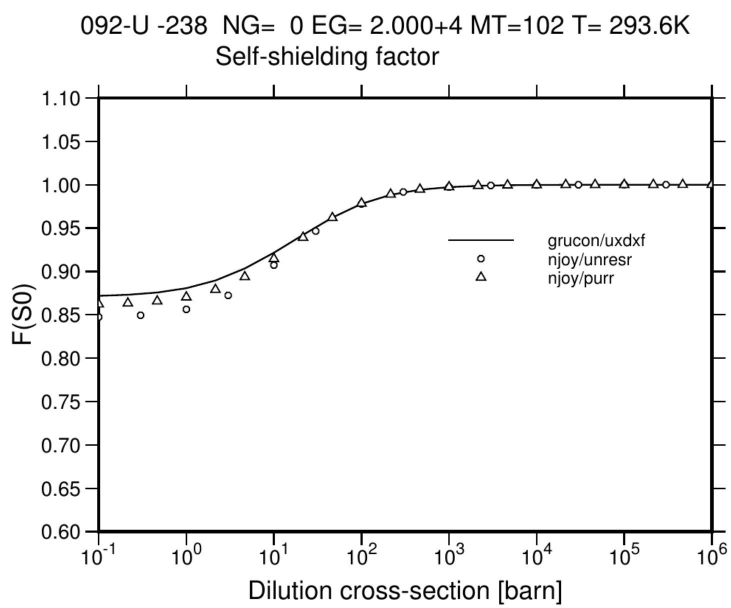




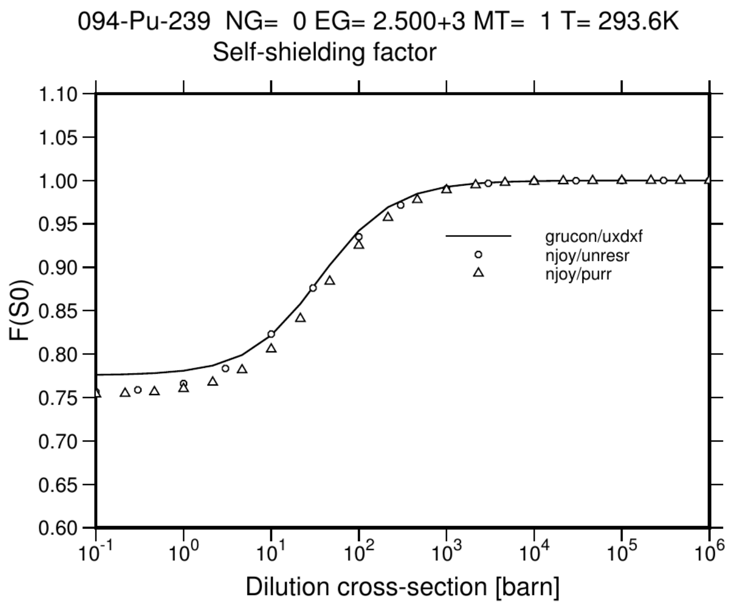
U-238 URR SS Factors: GRUCON/NJOY comparison

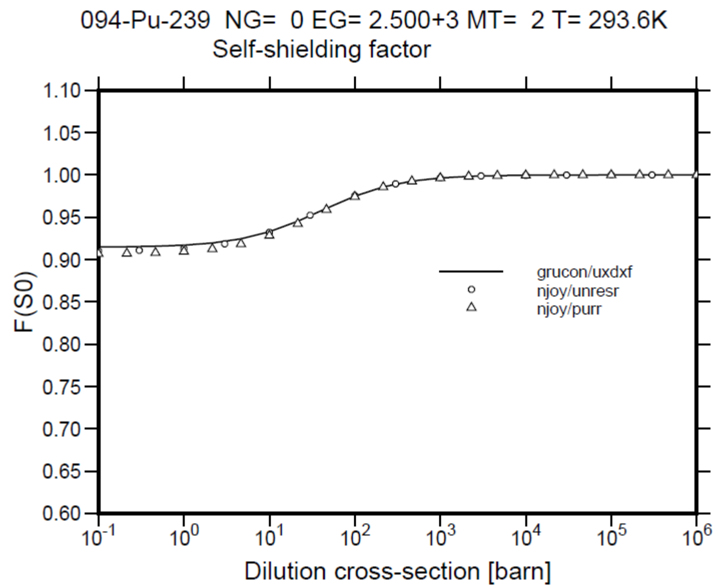


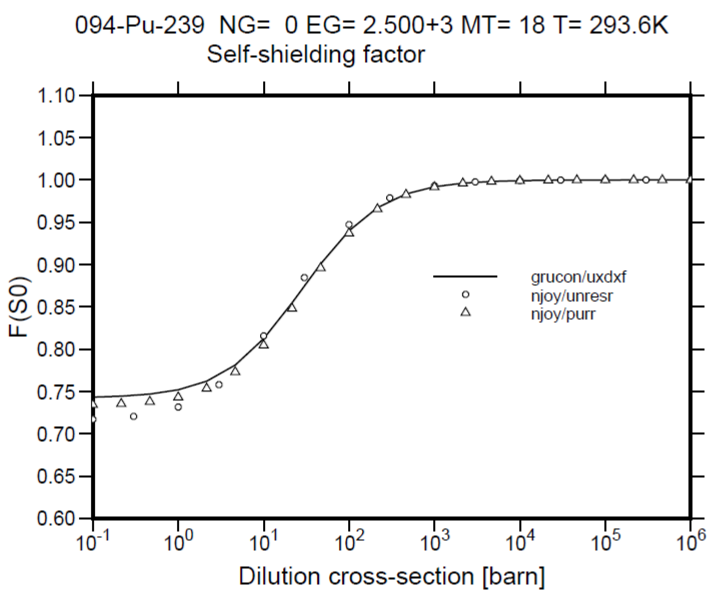


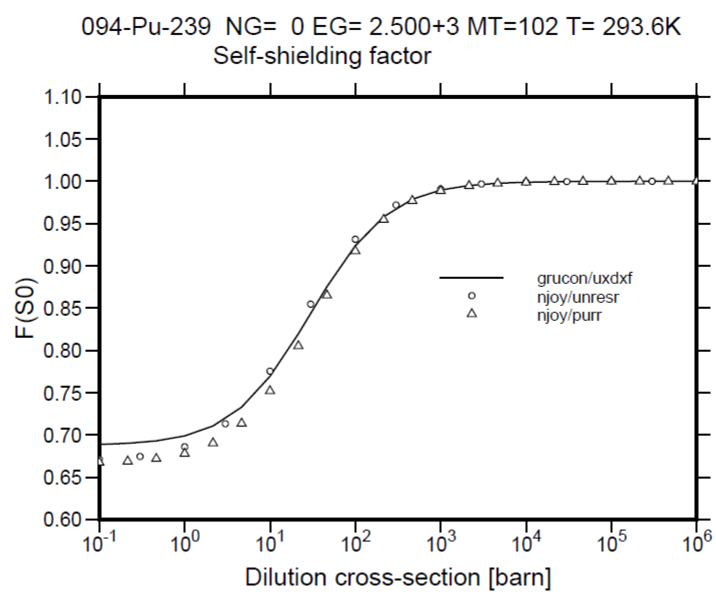


Pu-239 URR SS Factors: GRUCON/NJOY comparison









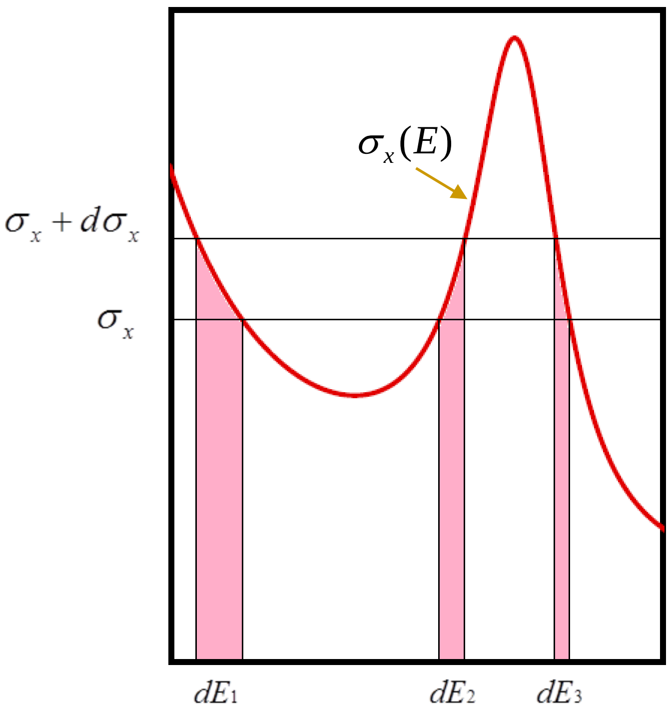
Probability Tables, Correlation Matrices and Subgroup Parameters (F/E-P, S/P-PN, PN/P-S, PN/PN-PC, PN/D-PC, P/C-P, P/D-F modules)

Probability Tables

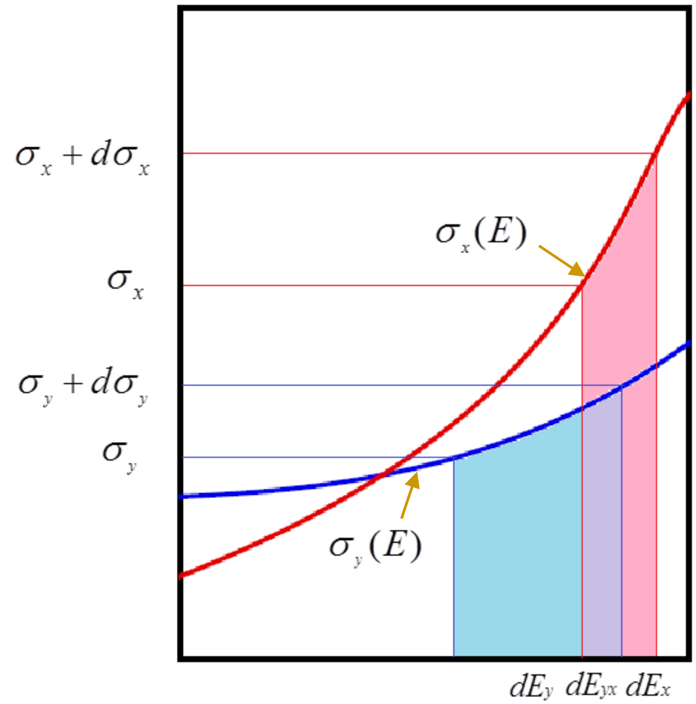
Correlation Matrices

"x","y" = {reaction, temperature, nuclide}

$$P(\sigma_x) = \sum_i \left| \frac{dE_i}{d\sigma_x} \right|$$



$$P(\sigma_y \mid \sigma_x)$$



Structural Parameters

$$P(\sigma_x) \sim \sum_{i=1}^{Nx} a_i^{(x)} \delta(\sigma_x - \sigma_i^{(x)})$$

$$P(\sigma_y \mid \sigma_x) \sim \sum_{j=1}^{Ny} \sum_{i=1}^{Nx} \omega_{j,i}^{(y,x)} a_i^{(x)} \delta(\sigma_x - \sigma_i^{(x)})$$

Physical constraints

$$\sum_{i=1}^{Nx} a_i^{(x)} = 1 \quad , \quad a_i^{(x)} > 0$$

$$\sigma_{\min}^{(x)} \le \sigma_i^{(x)} \le \sigma_{\max}^{(x)}$$

$$\sum_{j=1}^{Ny} \sum_{i=1}^{Nx} \omega_{j,i}^{(y,x)} = 1 \quad , \quad \omega_{j,i}^{(y,x)} \ge 0$$

Calculation of Subgroup Parameters

(Moments approximation with balance and normalization constraints)

Gauss approach

$$< (\sigma + \sigma_0)^n > = \sum_{i=1}^{N} a_i \, (\sigma_i + \sigma_0)^n$$

$$< \sigma_x(\sigma + \sigma_0)^n > = \sum_{i=1}^{N} a_i \sigma_{xi} \, (\sigma_i + \sigma_0)^n$$

$$\sum_{i=1}^{N} a_i = 1$$

$$\sum_{x} \sigma_{x\,i} = \sigma_i$$

Padé-II approximation

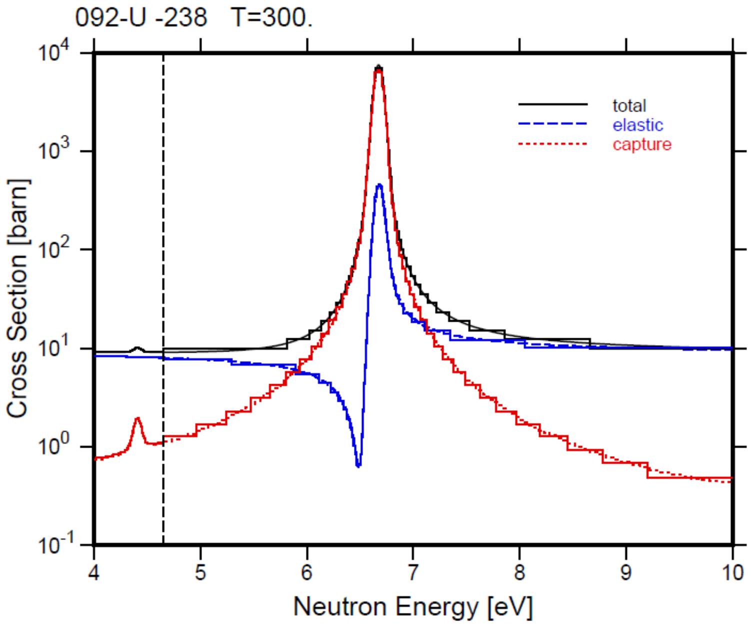
$$< 1/(\sigma + \sigma_{0j}) > \cong \sum_{i=1}^{N} a_i \, /(\sigma_i + \sigma_{0j})$$

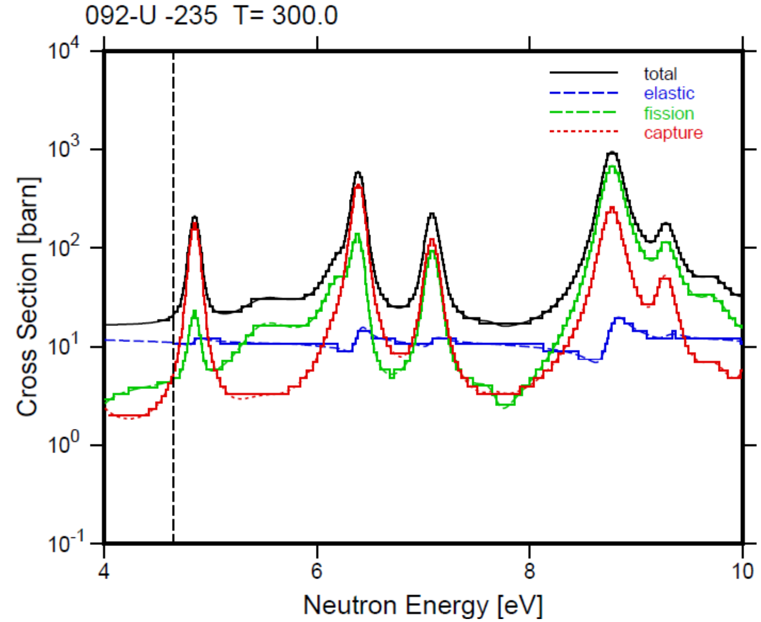
$$< \frac{\sigma_x}{\sigma + \sigma_{0j}} > \cong \sum_{i=1}^{N} a_i \sigma_{xi} \, /(\sigma_i + \sigma_{0j})$$

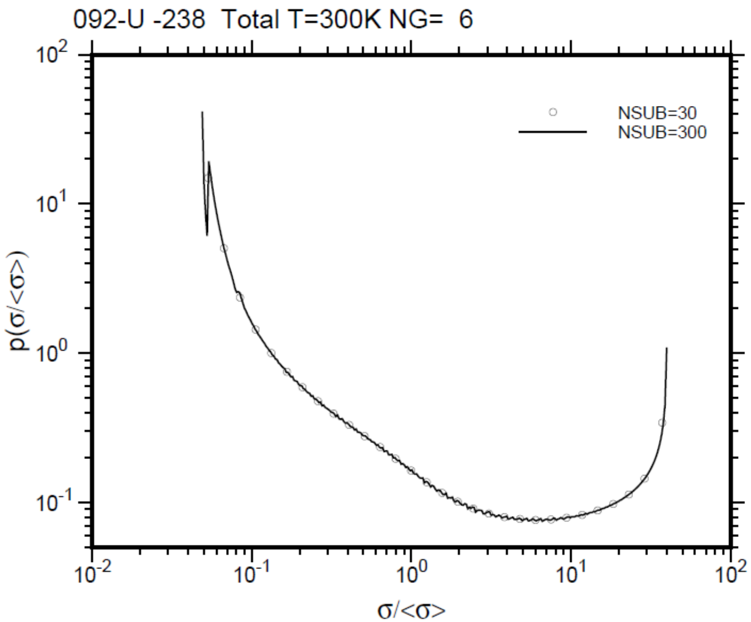
$$\sum_{i=1}^{N} a_i \sigma_i = < \sigma >$$

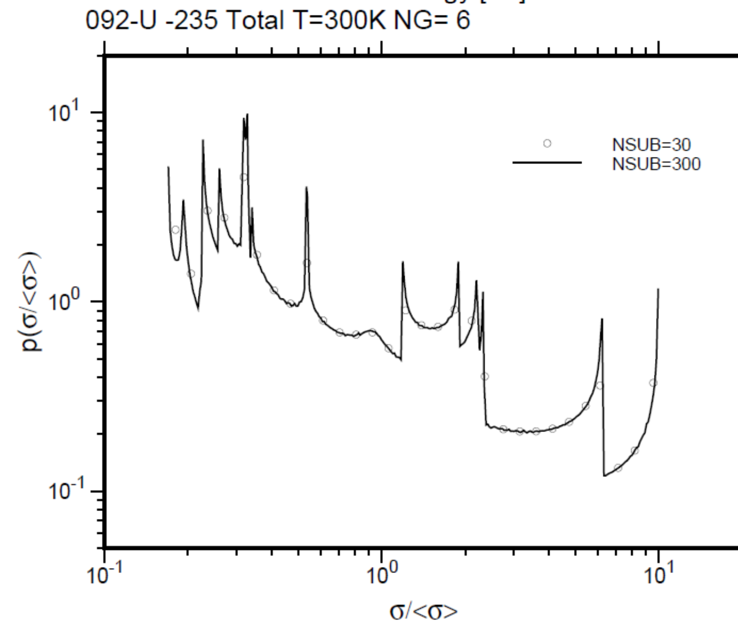
$$\sum_{i=1}^{N} a_i \, \sigma_{xi} = < \sigma_x >$$

Calculation of Probability Tables

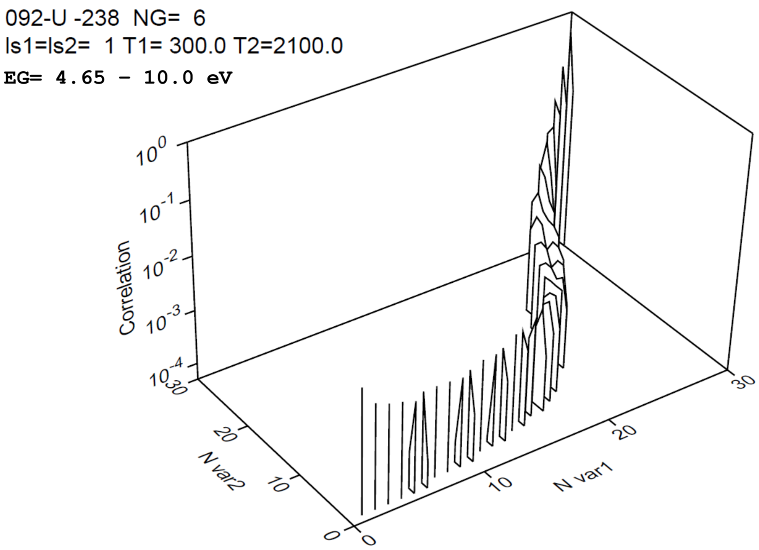


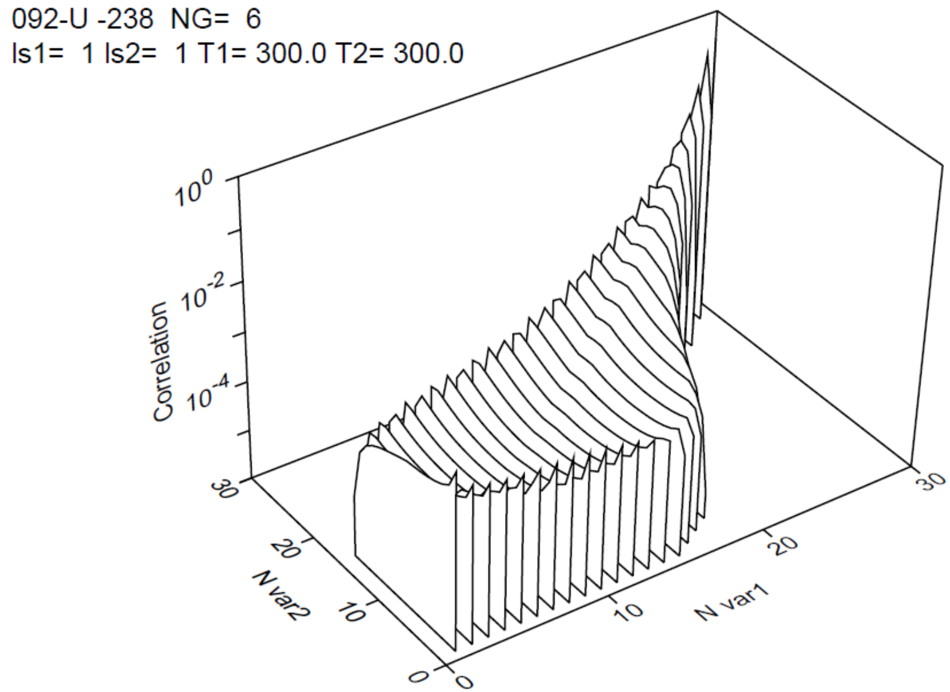


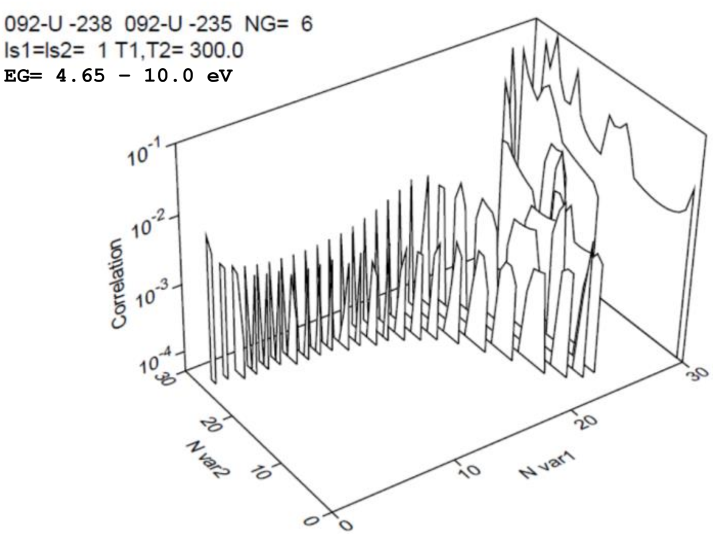




Correlation Matrices

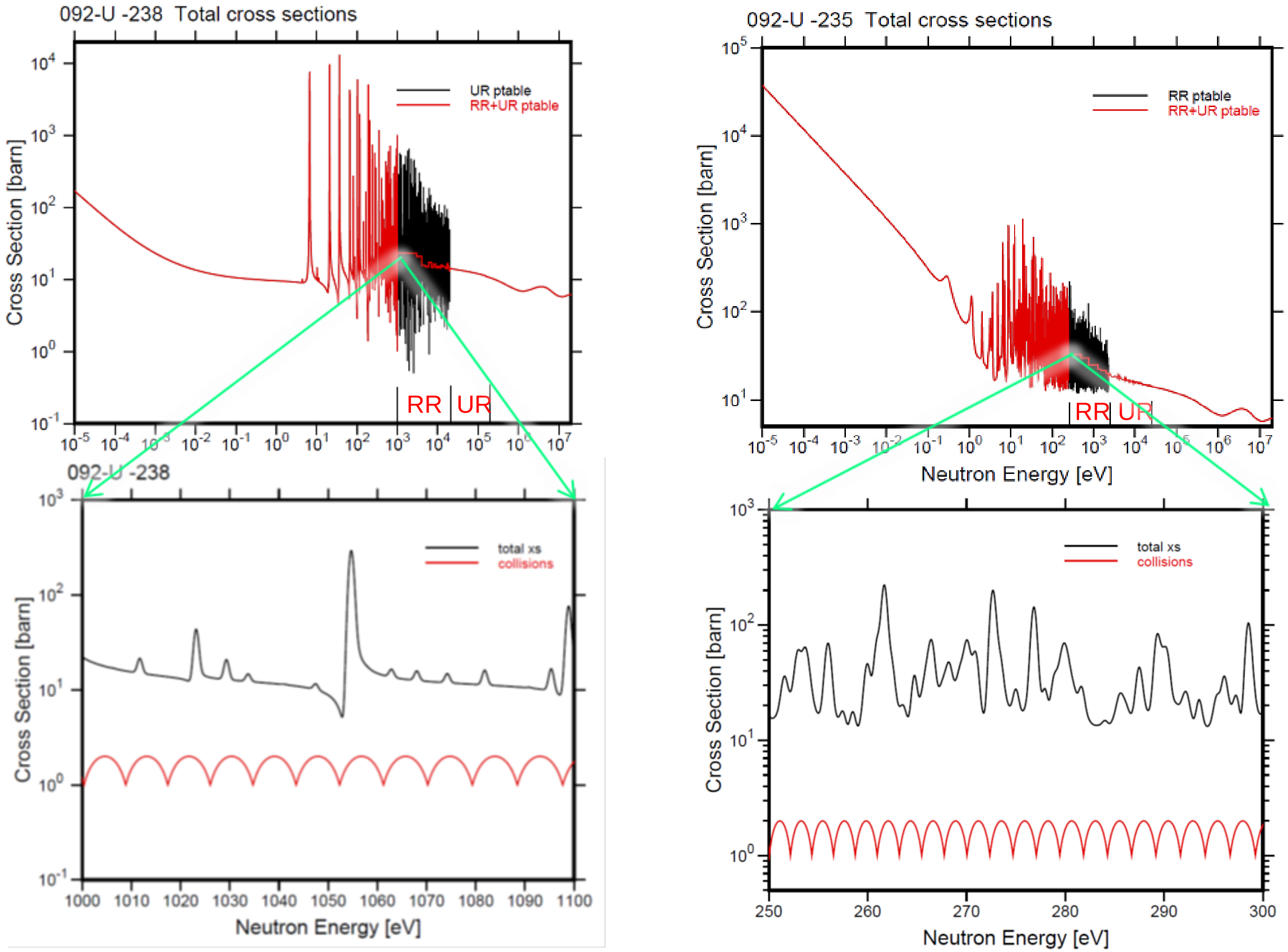






Appendix A. ACE files with Combined Probability Tables and Subgroup Parameters

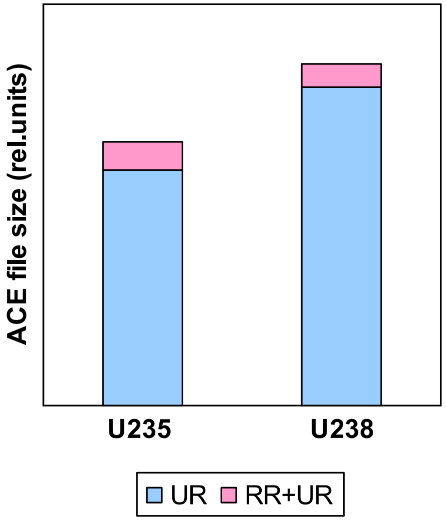
ACE files with Combined Probability Tables



Case A: subgroup parameters in URR
Case B: subgroup parameters in RRR & URR

Benchmark:

SCHERZO-556 - imaged critical infinity composition of 5.56% ^{235}U and 94.44% ^{238}U



	Experiment	A: UR	$(C_A/E-1)\%$	B: RR+UR	$(C_B/C_A-1)\%$
Kinf	1.000 ± 0.2%	1.0008±(1)	0.08	1.0009±(1)	0.01
F238/F235	0.0227 ± 1.3%	0.02234±(1)	-1.60	0.02233±(1)	-0.04
C238/F235	0.1154 ± 1.5%	0.11552±(3)	0.10	0.11552±(3)	0.00

Appendix B. ACE Files with Angular Distributions Reconstructed from Resonance Parameters (R/T-S, S/L-A, A/E-A modules)

Blatt-Biedenharn formalism:

$$d\sigma_{\alpha\alpha'}/\,d\Omega\ = \frac{\lambda_{\alpha}^{2}}{(2i+1)(2I+1)}\sum_{s,s'}\sum_{L=0}^{\infty} B_L(\alpha s, a's')P_L(\cos\theta)$$

$$B_L(\alpha s, a's') = \frac{(-1)^{s-s'}}{4}\sum_{J_1,J_2}\sum_{l_1,l_2}\sum_{l_1',l_2'} \overline{Z}(l_1 J_1 l_2 J_2\,|sL)\overline{Z}(l_1' J_1' l_2' J_2'|s'L)$$
$$\times\left(\delta_{\alpha\alpha'}\delta_{l_1 l_1'}\delta_{ss'} - U^{J_1}_{\alpha l_1 s,\alpha' l_1' s'}\right)\left(\delta_{\alpha\alpha'}\delta_{l_2 l_2'}\delta_{ss'} - U^{J_2}_{\alpha l_2 s,\alpha' l_2' s'}\right)$$

$$\overline{Z}(l_1 J_1 l_2 J_2|sL) = \sqrt{(2l_1+1)(2l_2+1)(2J_1+1)(2J_2+1)}\,(l_1 l_2 00|L0)W(l_1 J_1 l_2 J_2|sL)$$

Where $\overline{Z}$ is a Blatt-Biedenharn coefficients,
$W(l_1 J_1 l_2 J_2|sL)$ is a Racah coefficients,
$(l_1 l_2 00|L0)$ is a Clebsh-Gordan coefficients of angular momentum coupling,
and $U^{J_1}_{\alpha l_1 s,\alpha' l_1' s'}$ is a collision function.

Collision Matrix Calculation

Breight-Wigner approximation:

$$U_{cc'} = e^{-i(\varphi+\varphi')}\left(\delta_{cc'} + i\sum_{\lambda}\frac{\Gamma_{\lambda c}^{\frac{1}{2}}\omega_{\lambda cc'}\Gamma_{\lambda c'}^{\frac{1}{2}}}{E_\lambda + \Delta_\lambda - E - \frac{i\Gamma_\lambda}{2}}\right)$$

with

$\omega_{\lambda cc'} = 1$ (SLBW case) or

$$\omega_{\lambda cc'} = 1 + \sum_{\mu\neq\lambda}\left(\frac{\gamma_{\mu c}}{\gamma_{\lambda c}} + \frac{\gamma_{\mu c'}}{\gamma_{\lambda c'}}\right) \frac{\sum_{c''}\gamma_{\lambda c''}L_{c''}^{0}\gamma_{\mu c''}}{E_\mu+\Delta_\mu-E_\lambda-\Delta_\lambda-i\,(\Gamma_\mu-\Gamma_\lambda)/2} \quad \text{(MLBW case)}$$

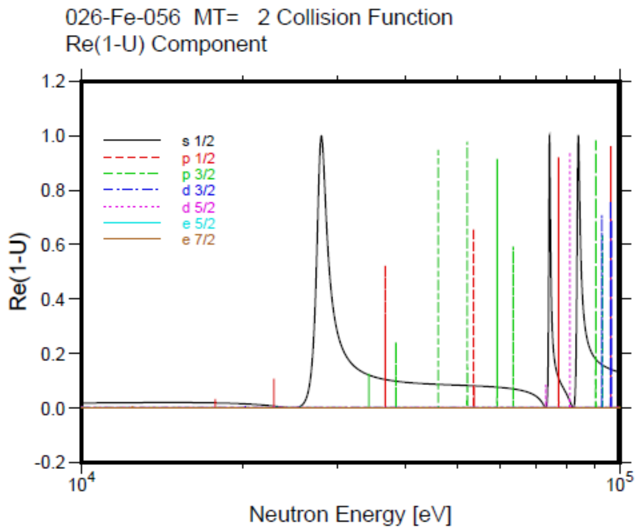
Reich-Moore approximation:

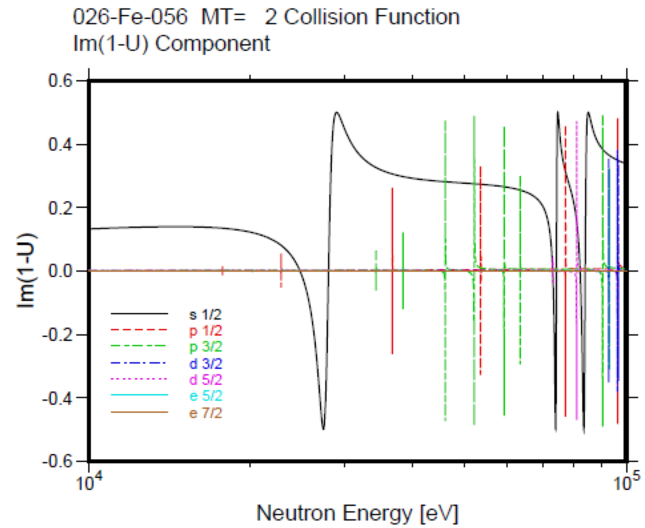
$$U_l = e^{-i2\varphi_l}\left(1 + \frac{2iR_lP_l}{1 - R_lL_l^0}\right)$$

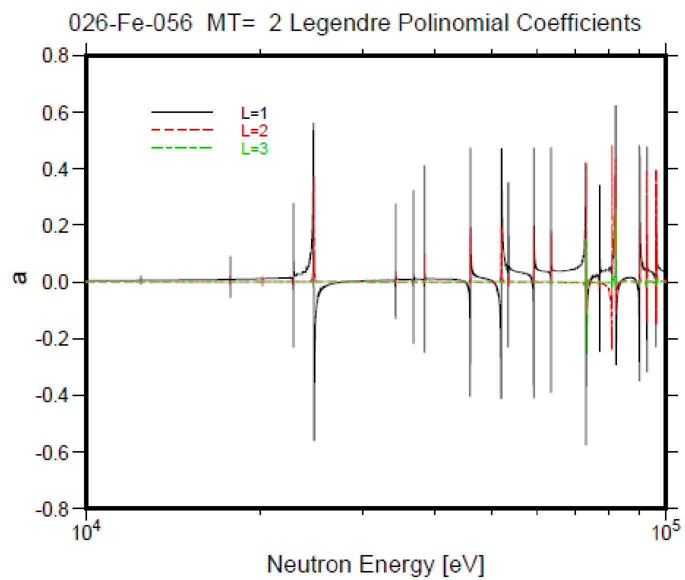
with R_l defined as

$$R_l \equiv \sum_{\lambda}\frac{\gamma_{\lambda l}^2}{E_\lambda - E - \frac{i\Gamma_{\lambda a}}{2}}$$

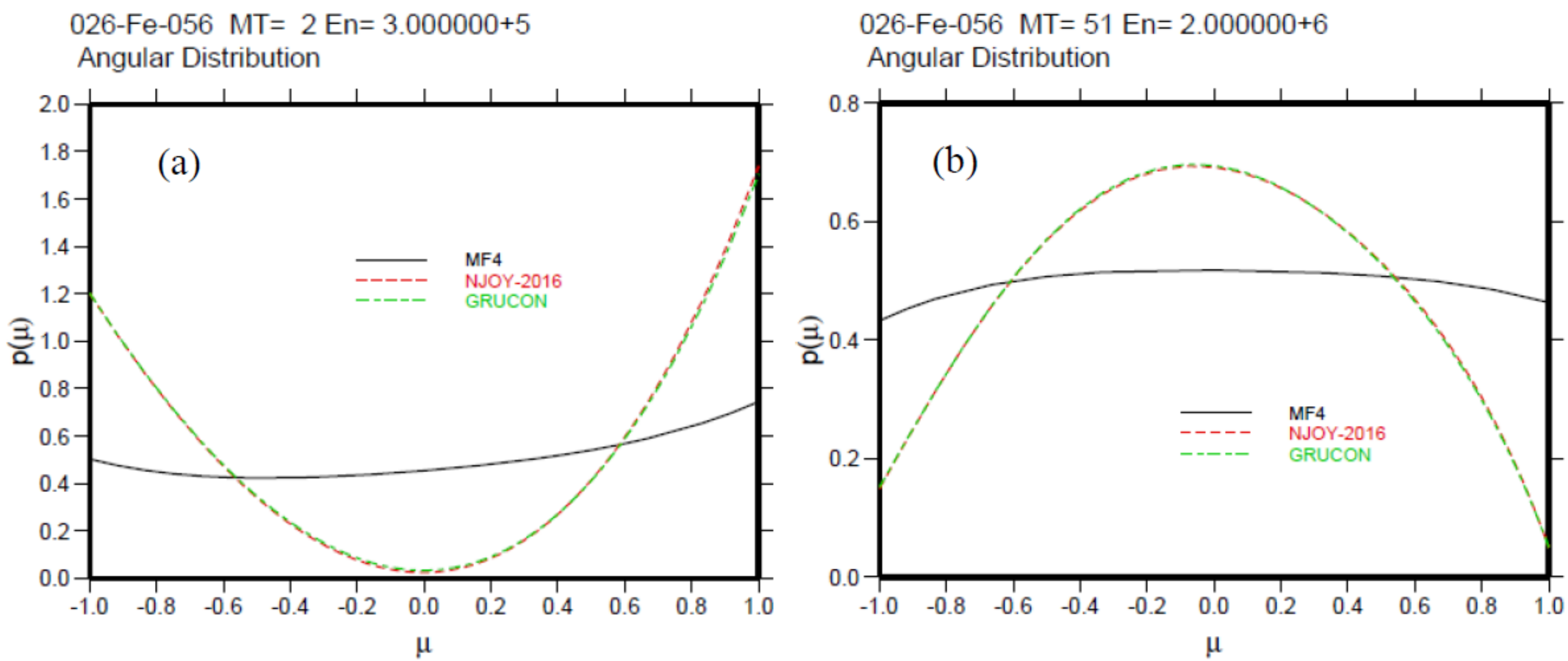
Collision function and Legendre polynomial coefficients







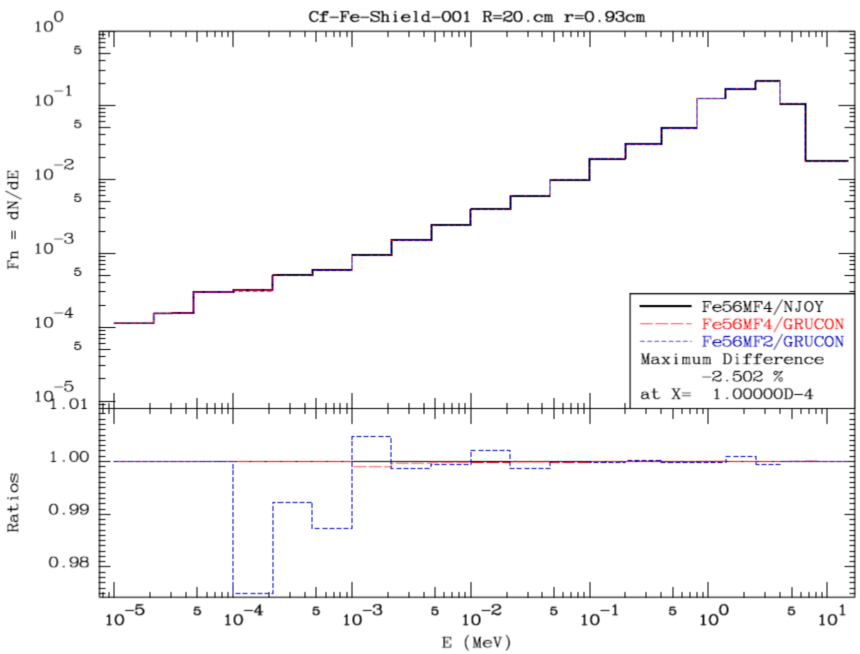
Comparison with NJOY and File Data



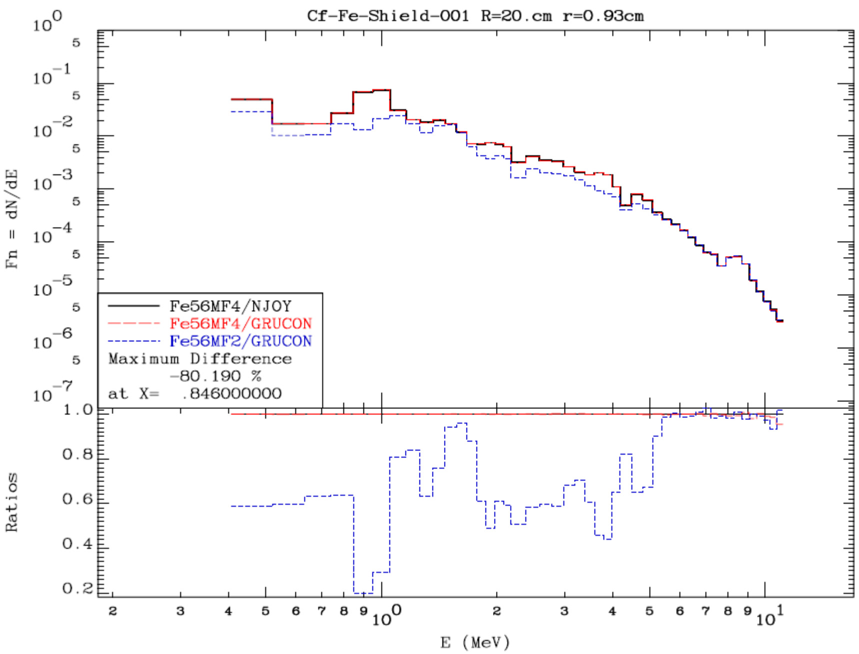
Leakage from Iron Shell with Cf-252 Source

(R=20cm r=0.93cm)

Neutrons



Photons



MF4 – angular distributions are taken from ENDF file

MF2 – angular distributions are restored from resonance parameters

Appendix C. Thermal ACE Files with Resonance Scattering Data (TH/-DS, S/T-DS module)

Neutron Scattering on Free Nuclei

Free gas approximation (Wigner-Wilkins - scattering cross section is constant) :

$$\sigma_s^T\left(E \to E', \vec{\Omega} \to \vec{\Omega}'\right) = \frac{\boldsymbol{\sigma_s}}{\boldsymbol{v}} \int_{allV:v_r>0} v_r\, P\left(v, V \to E', \vec{\Omega}'\right) M^T(V) dV$$

Scattering on resonances (Ouisloumen - Sanchez) :

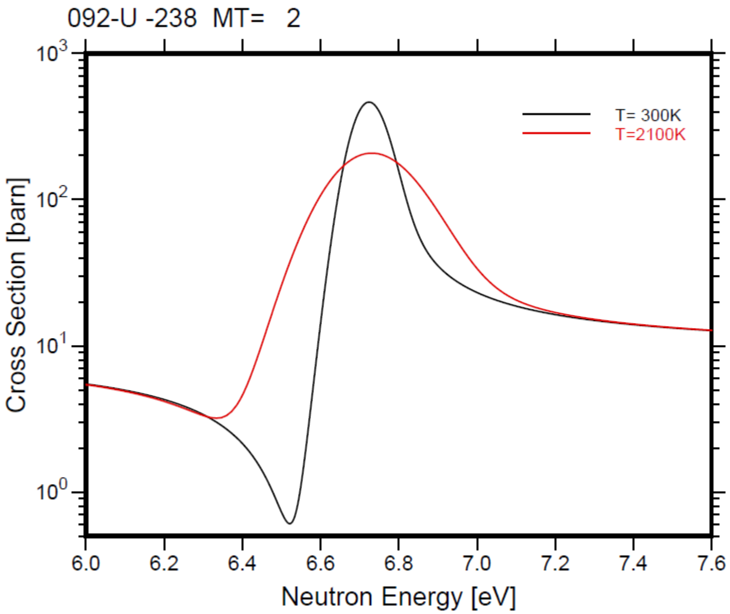
$$\sigma_s^T\left(E \to E', \vec{\Omega} \to \vec{\Omega}'\right) = \frac{1}{v} \int_{allV:v_r>0} v_r\, \sigma_s(v_r, 0) P\left(v, V \to E', \vec{\Omega}'\right) M^T(V) dV$$

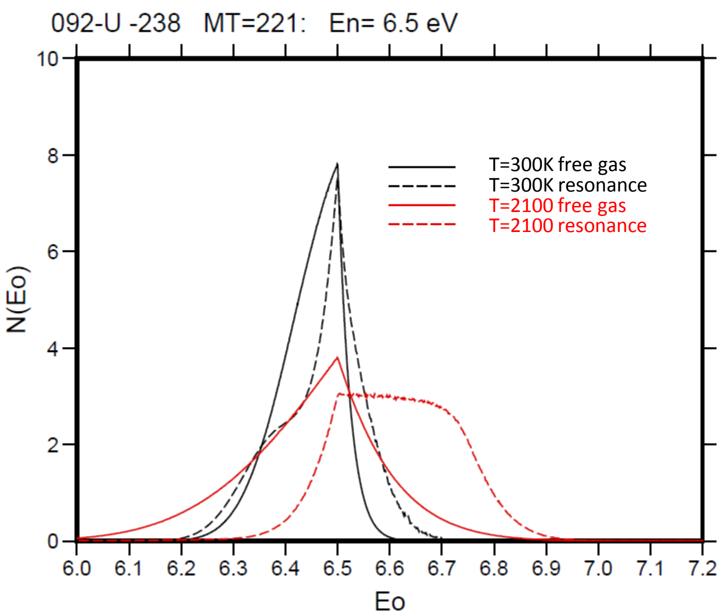
Where

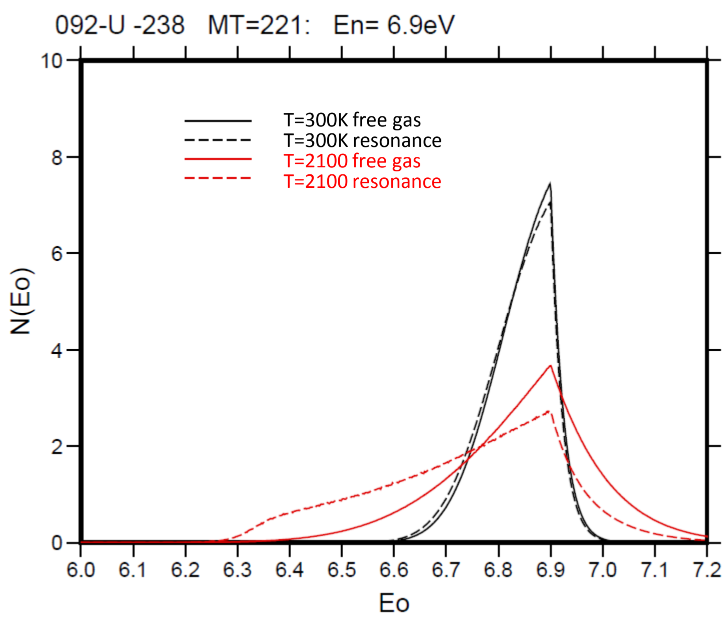
$P(V,T) = \frac{4}{\sqrt{\pi}} \beta^{3/2} V^2 e^{\left(-\beta V^2\right)}$ - Maxwell-Boltzmann distribution

Scattering on the U-238 Resonance

Neutron spectra on the left (En=6.5eV) and the right (En=6.9eV) wings of U-238 resonance, calculated in free gas and resonance scattering models







ACE Files for Thermal Neutrons with Resonance Scattering Data

Mosteller Benchmark Specification

Task – calculate Doppler coefficient of reactivity $DC = \frac{\Delta\rho_{Dop}}{\Delta T_{Fuel}}$

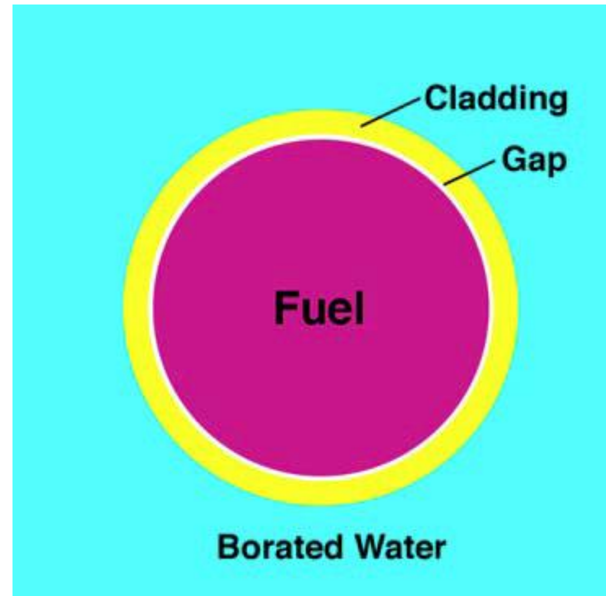
where $\Delta\rho_{Dop} = \frac{k_{HFP} - k_{HZP}}{k_{HFP} \times k_{HZP}}$ - Doppler defect

ΔT_{Fuel} - difference of fuel temperatures for conditions:

HZP – hot zero power (600K)

HFP – hot full power (900K)

Schematic of the Geometry



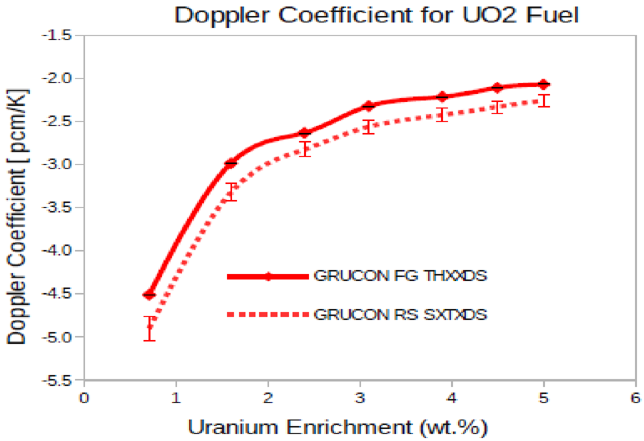
Subsets of benchmarks:

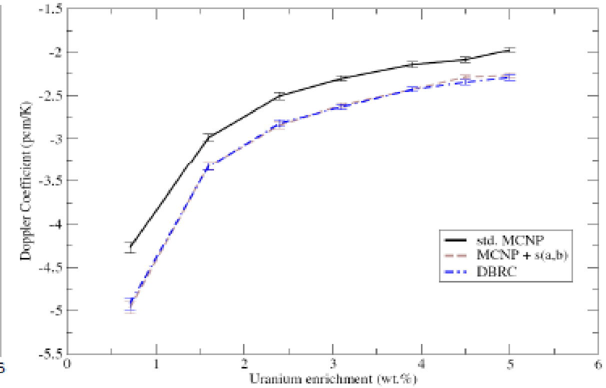
- UO2, fuel, ranging from normal to 5 wt. % enriched uranium
- Reactor–Recycled MOX (UO2+PuO2), PuO2 from 1 wt. % to 8 wt. %
- Weapons-Grade MOX (UO2+PuO2), PuO2 from 1 wt. % to 6 wt. %

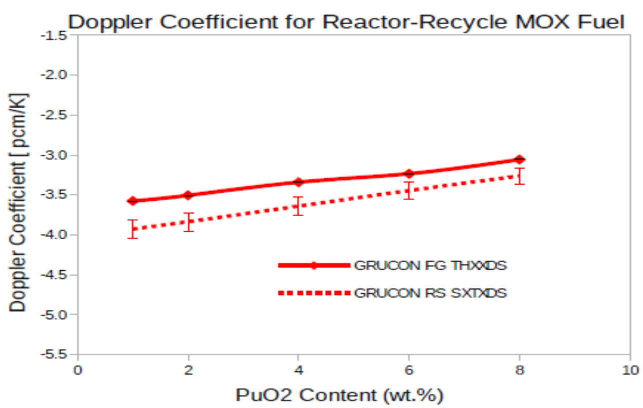
Moderator: Water + B (1400 ppm) , T=600K

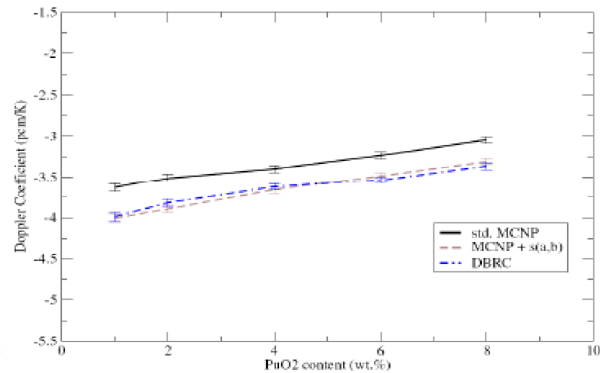
Cladding: Zr, T=600K

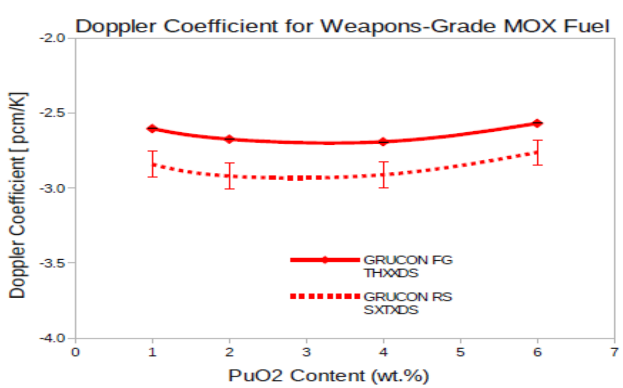
Resonance Scattering Effect

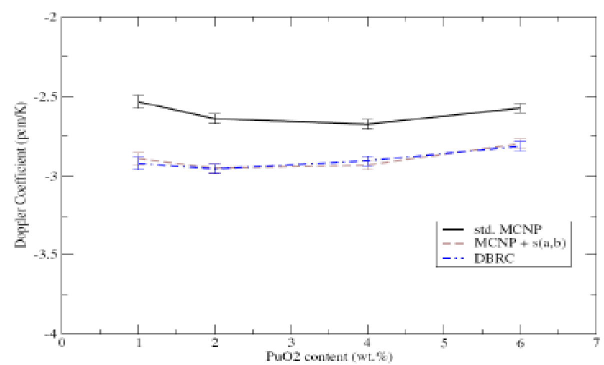












B.Becker, R.Dagan, C.H.M.Broeders, G.Lohnert, ”An Alternative Stochastic Doppler Broadening Algorithm”, M&C, Saratoga Springs, New York, May 3-7, 2009

Acknowledgments

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Thank You for Attention!